

# Stripe order in the underdoped region of the two-dimensional Hubbard model

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**Competing inhomogeneous orders are a central feature of correlated electron materials including the high-temperature superconductors. The two-dimensional Hubbard model serves as the canonical microscopic physical model. Multiple orders have been proposed in the underdoped part of the phase diagram, which corresponds to a regime of maximum numerical difficulty. By combining the latest numerical methods in exhaustive simulations, we provide a definitive resolution of the order in the underdoped ground state. We find a stripe order that is highly compressible near full filling on an energy scale of a few Kelvin, with wavelength fluctuations coupled to pairing order. Additional**

**physics beyond the Hubbard model is now necessary to account for deviations from this picture. Our results demonstrate the power of modern numerical methods to solve microscopic models even in the most challenging settings.**

## Introduction

Competing inhomogeneous orders are a common feature in many strongly correlated materials (1). A famous example is found in the underdoped region of the phase diagram of the high-temperature cuprate superconductors (HTSC). Here, multiple probes, including neutron scattering, scanning tunneling microscopy, resonant X-ray scattering, and nuclear magnetic resonance spectroscopy all lend support to various proposed inhomogeneous orders, such as charge, spin, and pair density waves, with suggested patterns ranging from unidirectional stripes to checkerboards (2, 3). Recent experiments on cuprates indicate that the observed inhomogeneous orders are distinct from, and compete with, pseudogap physics (4, 5).

Much theoretical effort has been directed to explain the origin of the inhomogeneities (6). Numerical calculations on microscopic lattice models have provided illuminating examples of the possible orders. The prototypical lattice model to understand HTSC is the 2D Hubbard model on the square lattice, with the Hamiltonian

$$H = - \sum_{\langle ij \rangle, \sigma \in \{\uparrow, \downarrow\}} t a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

where  $a^{(\dagger)}$  and  $n$  denote the usual fermion creation, annihilation, and number operators, and  $t$  and  $U$  are the kinetic and repulsion energies. A large number of numerical techniques have been applied to compute the low-temperature and ground-state phase diagram of this model. Early evidence for unidirectional stripe ordering in the Hubbard model came from Hartree-Fock calculations (7–10), while non-convex energy versus filling curves in exact diagonalization of small clusters of the related  $t$ - $J$  model were interpreted as signs of macroscopic

phase separation (11, 12). Since then, inhomogeneous orders have been observed both in the Hubbard and  $t$ - $J$  models with density matrix renormalization group (DMRG) (13–15), variational quantum Monte Carlo (16) and constrained path auxiliary field quantum Monte Carlo (AFQMC) (17), infinite projected entangled pair states (iPEPS) (18), density matrix embedding theory (DMET) (19), and functional renormalization group (20) calculations amongst others, although not necessarily the same kind of inhomogeneity is observed in each case. However, there are other sophisticated simulations, for example, with variational and projector quantum Monte Carlo (21, 22), and cluster dynamical mean-field theory, which do not see, or are unable to resolve, the inhomogeneous order (23, 24). The most recent studies with iPEPS (18) and DMET (19), as well as some earlier variational calculations (16, 25–27), further show that both homogeneous and inhomogeneous states can be observed and stabilized within the same numerical methodology, with a small energy difference between homogeneous and inhomogeneous states, on the order of  $\sim 0.01t$  per site.

The small energy differences between orders means that very small biases in ground state simulations, such as from an incomplete treatment of fluctuations, using insufficiently accurate constraints to control the sign problem, or from finite size effects, can easily stabilize one order over the other. Similarly, the low temperatures needed to resolve between orders is a challenge for finite temperature methods (28, 29). Settling the resulting debate between candidate states has thus so far been beyond reach. However, in this work we will demonstrate that, with the latest numerical techniques, obtaining a *definitive* characterization of the ground state order in the underdoped region of the 2D Hubbard model is now an achievable goal. As a representative point in the phase diagram, we choose the iconic  $1/8$  doping point at strong coupling ( $U/t = 8$ ). Experimentally, this doping corresponds to a region of maximal inhomogeneity in many HTSC's, and in the strong coupling regime it is recognized as a point of maximum numerical difficulty and uncertainty in simulations (24). Using state-of-the-art computations with

detailed cross-checks and validation, including newer methodologies such as infinite projected-entangled pair states (iPEPS) and density matrix embedding theory (DMET) as well as recent developments in established methodologies such as constrained-path auxiliary field quantum Monte Carlo (AFQMC) and density matrix renormalization group (DMRG), and with exhaustive accounting for finite size effects combined with calculations directly in the thermodynamic limit, we are able to achieve unprecedented accuracy in this challenging region of the ground-state phase diagram. In so doing, we can finally answer the question: what is the order and physics found in the underdoped ground state of the 2D Hubbard model?

## Computational strategy

An important new strategy we bring to bear on this part of the Hubbard model phase diagram is to combine the insights of multiple numerical tools with complementary strengths and weaknesses. This approach, pioneered in an earlier work involving some of us (24), greatly increases the confidence of the numerical characterization. To understand what each method contributes, we briefly summarize the theoretical background and corresponding sources of error. Further details are provided in the SI.

*Auxiliary field quantum Monte Carlo.* AFQMC expresses the ground state of a finite system through imaginary time evolution,  $\lim_{\beta \rightarrow \infty} e^{-\beta H} |\Phi_0\rangle$ , where  $|\Phi_0\rangle$  is an initial state. The projection is Trotterized, and the evolution reduces to a stochastic single-particle evolution in the presence of auxiliary fields generated by the Hubbard-Stratonovich decoupling of the Hubbard repulsion. Away from half-filling, this decoupling has a sign problem. We use the constrained path (CP) approximation, to eliminate the sign problem at the cost of a bias dependent on the quality of the trial state (30, 31). In this work, the Trotter error is well converged and we report the statistical error bar. To minimize the constrained path bias, we use several different trial states, including self-consistent optimization of the trial state (32). The calculations are carried

out on finite cylinders with open, periodic, and twist-averaged boundary conditions, with widths of up to 12 sites, and lengths of up to 72 sites. This method can reach large sizes and finite size effects are minimized. The uncontrolled error is from the CP approximation.

*Density matrix renormalization group.* DMRG is a variational wavefunction approximation using matrix product states (MPS), which are low-entanglement states with a 1D entanglement structure. The quality of the approximation is determined by the bond dimension of the MPS. The calculations are carried out on finite cylinders with widths of up to 7 sites, and lengths of up to 64 sites, with periodic boundary conditions in the short direction and open boundaries in the long direction. Two different DMRG algorithms were used: one working in a pure (real-space) lattice basis, and another in a mixed momentum/lattice (hybrid) basis, with the momentum representation used along the short periodic direction (33). We remove the bond dimension error and finite size error in the long direction by well-known extrapolation procedures, and report the associated error bar (34). Consistency between the lattice and hybrid DMRG algorithms provides a strong validation of this error bar. The remaining uncontrolled error is the finite width error in the periodic direction.

*Density matrix embedding.* DMET is a quantum embedding method which works directly at the thermodynamic limit, although interactions are only accurately treated within an impurity cluster (35). To solve the impurity problem, consisting of a supercell of the original lattice coupled to a set of auxiliary bath sites, we use a DMRG solver. We treat supercells with up to 18 sites. The error bar reported in DMET corresponds to the estimated error from incomplete self-consistency of the impurity problem. The remaining uncontrolled error is the finite impurity size error.

*Infinite Projected Entangled Pair states.* iPEPS is a variational approach using a low-entanglement tensor network ansatz natural to 2D systems (36–38). The calculations are carried out directly in the thermodynamic limit where different supercell sizes including up to 16 sites are used

to target different low-energy states. As in DMRG, the accuracy of the ansatz is systematically controlled by the bond dimension  $D$  of the tensors. Estimates of quantities in the exact  $D$  limit are obtained using an empirical extrapolation technique which is a potential source of uncontrolled error.

*Cross-checks: systematic errors, finite size biases.* The use of multiple techniques allows us to ameliorate the uncontrolled errors from one technique using information from another. For example, by carrying out simulations on the same finite clusters in the AFQMC and DMRG calculations, we can estimate the constrained path bias in AFQMC. Similarly, in the AFQMC calculations we can treat larger width cylinders than in the DMRG simulations; thus we can estimate the finite width error in DMRG.

In all of the methods, there is a bias towards orders commensurate with the shape of the simulation cell, be it the finite lattice and boundary conditions in AFQMC/DMRG, or the impurity cluster in DMET, or the supercell in iPEPS. Using this bias, together with different boundary conditions and pinning fields, we can stabilize different *meta-stable* orders. For example, by setting up clusters commensurate with multiple inhomogeneous orders and observing the order that survives, we can determine the relative energetics of the candidate states. We can fit the orders along the short axis or the long axis of the cluster to obtain two independent estimates of the energy. We have carried out exhaustive studies of about 100 different combinations of clusters, cells, and boundary conditions, to fully investigate the low-energy landscape of states. These detailed results are presented in the SI. To characterize the orders, we use the local hole density  $1 - (\langle n_{\uparrow} + n_{\downarrow} \rangle)$ , magnetic moment  $\frac{1}{2} \langle n_{\uparrow} - n_{\downarrow} \rangle$ , and pairing order  $\frac{1}{\sqrt{2}} (a_{i\uparrow}^{\dagger} a_{j\downarrow}^{\dagger} + a_{j\uparrow}^{\dagger} a_{i\downarrow}^{\dagger})$  ( $i$  adjacent to  $j$ ).

## Characterizing the ground state at 1/8 doping

Using the above methods, we carried out calculations for the ground state of the 2D Hubbard model at 1/8 doping at  $U/t = 8$ . The first check of reliability is the independent convergence of the methods for the energy per site. While the quality of the ground-state energy may be a poor proxy for the quality of the corresponding state when the overall accuracy is low (as there are always many degenerate states far above the ground state) well-converged energies are a much tighter constraint on the ground state order, as any degeneracies must be below the energy convergence threshold. Fig. 1 shows the best energy estimate for the ground state from the different methods. The two different DMRG formulations (real-space and hybrid basis) agree perfectly, providing a strong independent check of the calculations, and in subsequent figures we report only the single consistent result. Note that the error bars for AFQMC, DMRG, and DMET, do not reflect the uncontrolled systematic errors in the methods. However, as described above, the systematic errors can be estimated by cross-checks between the methods. For example, DMRG and AFQMC calculations on finite clusters with identical boundary conditions provide an estimate of the small constrained path bias (see SI and Ref. (32)) consistent with the difference in the DMRG and AFQMC energies in Fig. 1; similarly AFQMC extrapolations to the thermodynamic limit indicate that the DMRG energies are essentially converged with respect to cylinder width.

There is close agreement between all the methods, and all energies lie in the range  $-0.767 \pm 0.004t$ . If, for a typical HTSC material, we estimate  $t \sim 3000K$ , then this corresponds to a range of about  $\pm 10K$  per site, or  $\pm 100K$  per hole. For a numerical comparison, this is also more than an order of magnitude lower than the temperatures accessible in finite temperature, thermodynamic limit, simulations in this part of the phase diagram, indicating that we are potentially accessing different physics (24, 29). Shown in the inset are the corresponding best estimates

at half-filling from the same methods, where the spread in energies is less than  $0.001t$ . This illustrates the significantly greater numerical challenge encountered in the underdoped region. Nonetheless, the accuracy and agreement reached here represents a ten-fold improvement over recent comparisons of numerical methods at this point in the phase diagram (24).

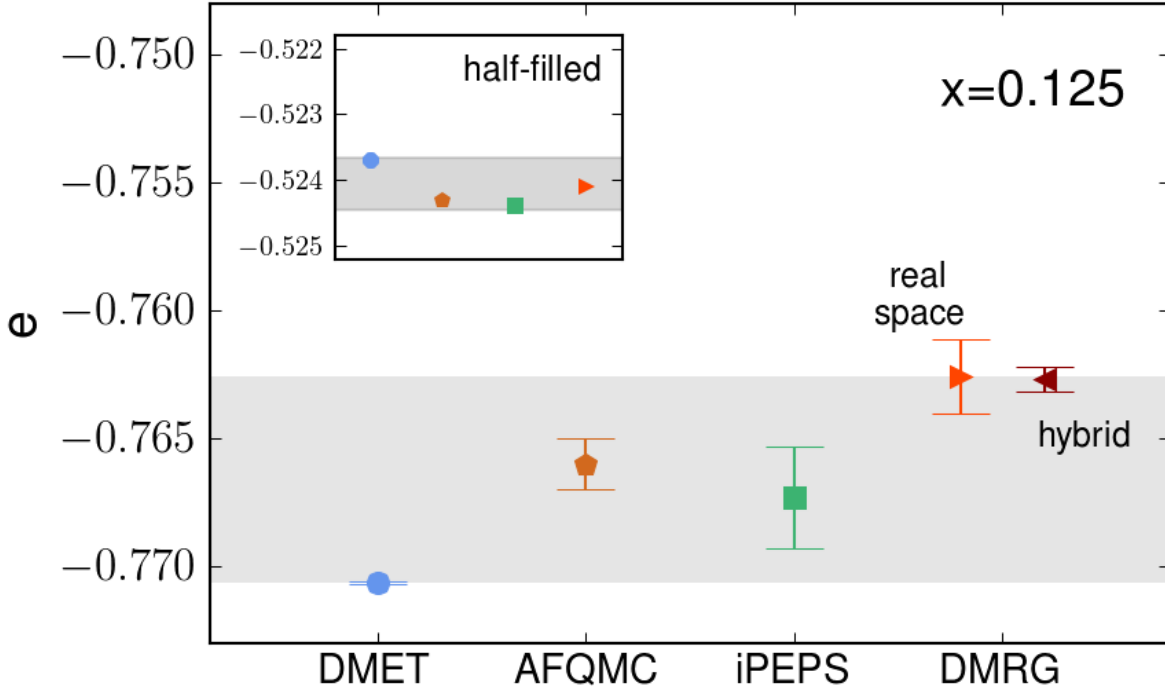


Figure 1: Best estimates of ground state energy for the 1/8-doped 2D Hubbard model at  $U/t = 8$  from DMET, AFQMC, iPEPS and DMRG. Inset: Best estimates of ground state energy for the half-filled 2D Hubbard model at  $U/t = 8$ .

*Ground state stripe order.* For all the methods employed, the lowest energies shown in Fig. 1 correspond to a *vertical striped state*. This corresponds to a co-directional charge and spin-density wave, with the region of maximum hole density coinciding with a domain wall in the antiferromagnetism. As mentioned, unidirectional stripes of various kinds are a long-standing candidate order in the doped Hubbard and related models. Hartree-Fock calculations give filled stripes (i.e. one hole per charge unit cell) in both vertical and diagonal orientations, while one



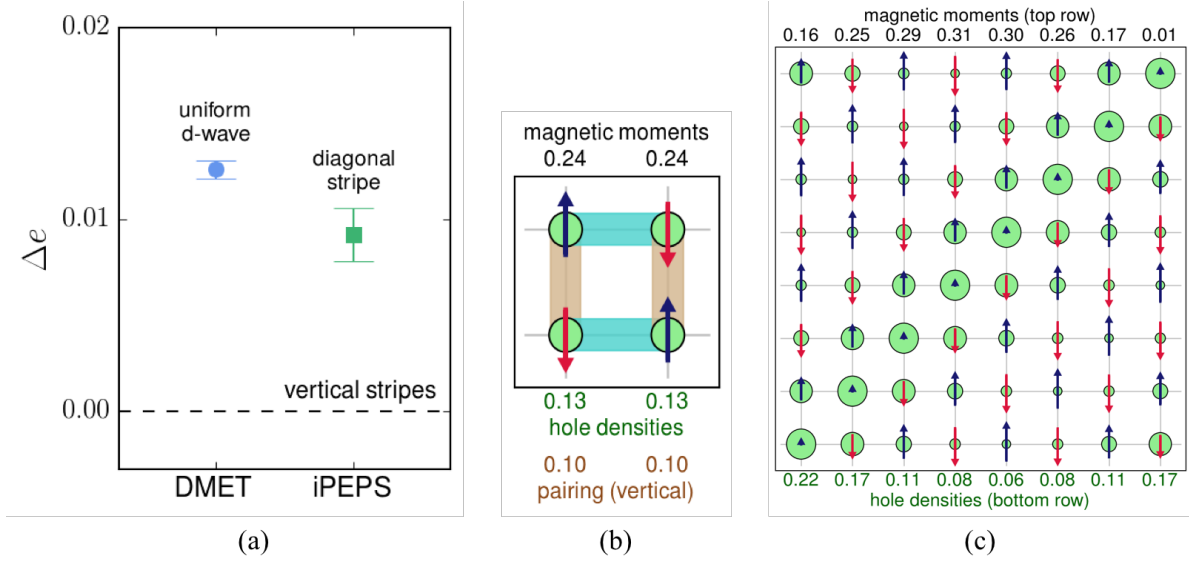


Figure 2: Energies of important competing states relative to the striped ground state from DMET and iPEPS and the orders. (a) Relative energy of competing states compared to the vertical striped state. (b) Charge, spin and pairing orders of the uniform  $d$ -wave state from DMET. (c) Charge and spin orders of the diagonal striped state from iPEPS. Note that the spins are flipped in the neighboring supercells. (Circle radius is proportional to hole density, arrow height is proportional to spin density, bond width is proportional to pairing density).

of the first applications of the DMRG to 2D systems found strong evidence for half-filled stripes in the  $t$ - $J$  model (13). Finally, one of the earliest examples of inhomogeneity in doped HTSC's were the static half-filled stripes in LaSrCuO at 1/8 doping (39).

The convergence to the same inhomogeneous order in the ground state in the current study, from multiple methods with very different approximations, strongly suggests that stripes indeed represent the true ground state order of the Hubbard model in the underdoped regime, and further highlights the accuracy we achieve with different techniques. However, the stripe order we observe has some unusual characteristics. We return to the details of the stripe order, its associated physics, and its relationship with experimentally observed stripes further below. First, however, we examine the possibility of other competing meta-stable states.

*Competing states: uniform  $d$ -wave state.* Recent work using iPEPS and DMET on the  $t$ - $J$  and Hubbard models suggested close competition between a uniform  $d$ -wave superconducting ground state and a striped order (18, 19). Uniform states did not spontaneously appear in any of our calculations which indicates that they lie higher in energy than the striped order. We found that we could stabilize a uniform  $d$ -wave state in the DMET calculations by constraining the impurity cluster to a  $2 \times 2$  or  $2\sqrt{2} \times \sqrt{2}$  geometry; similarly shaped larger clusters (such as a  $4 \times 4$  cluster) spontaneously broke symmetry to create a non-uniform state. From these calculations we estimate that the uniform state lies  $\sim 0.01t$  above the lowest energy state, and is not competitive at the energy resolution we can now achieve.

*Competing states: other short-range orders.* While other types of order have been proposed in the underdoped region, such as spiral magnetic phases (20, 40) and checkerboard order (41), we find no evidence for other kinds of short-range orders at this point in the phase diagram. The lack of checkerboard order, which would easily fit within the large clusters in our simulations (e.g. up to  $64 \times 6$  in the DMRG calculations) appears to rule them out as low energy states, in agreement with earlier DMRG simulations on the  $t$ - $J$  model (42). While we cannot rule out in-

commensurate orders, we have found that the variation of energy with unit cell wavelength (see below) is quite smooth, thus we do not expect a dramatic energy gain from incommensurability. We note that studies finding incommensurate magnetic orders have focused on smaller values of  $U$  (20).

*Diagonal versus vertical stripes.* While we find the ground state order to be a vertical stripe type order, other studies of stripes indicate that different orientations can form (43). On short length scales, the relevant question is whether diagonal stripes (with a  $(\pi, \pi)$  wave vector) are competitive with vertical stripes (with a  $(0, \pi)$  wavevector). With the boundary conditions used in this work, diagonal stripes would be frustrated in the DMRG and AFQMC calculations, and did not spontaneously appear. To stabilize diagonal stripes in the DMET and iPEPS calculations, we used tilted  $n\sqrt{2} \times \sqrt{2}$  impurity clusters ( $n = 2, 5$ ) for DMET, and a  $16 \times 16$  simulation cell with 16 independent tensors in iPEPS. The  $16 \times 16$  iPEPS cell gave a diagonal stripe (Fig. 2) that was significantly higher in energy than the vertical stripe, by  $0.009t$ . The DMET cluster gave rise to a frustrated diagonal order that we also estimate to be higher in energy by  $\sim 0.005t$  (see SI). While it is likely that the orientation of the stripe will depend on doping and coupling, vertical stripes appear to be significantly preferred at this point in the phase diagram.

*Ground state stripes: detailed analysis.* We now return to a more detailed discussion of the vertical stripe order observed in the ground-state. Within the family of vertical stripes, we can consider questions of wavelength (charge and spin periodicity), type and strength of charge and spin modulation (e.g. bond- versus site-centered), and coexistence with pairing order.

We first discuss the wavelength  $\lambda$ . At  $1/8$  doping, the filling of the stripe is related to the wavelength by  $\lambda/8$ . As described, we can access different wavelength meta-stable stripes and their relative energetics by carefully choosing different total cluster dimensions and boundary conditions (in the DMRG and AFQMC calculations) or unit cell/impurity sizes (in the iPEPS and DMET calculations). Fig. 3 shows the energy per site of the stripe versus its wavelength

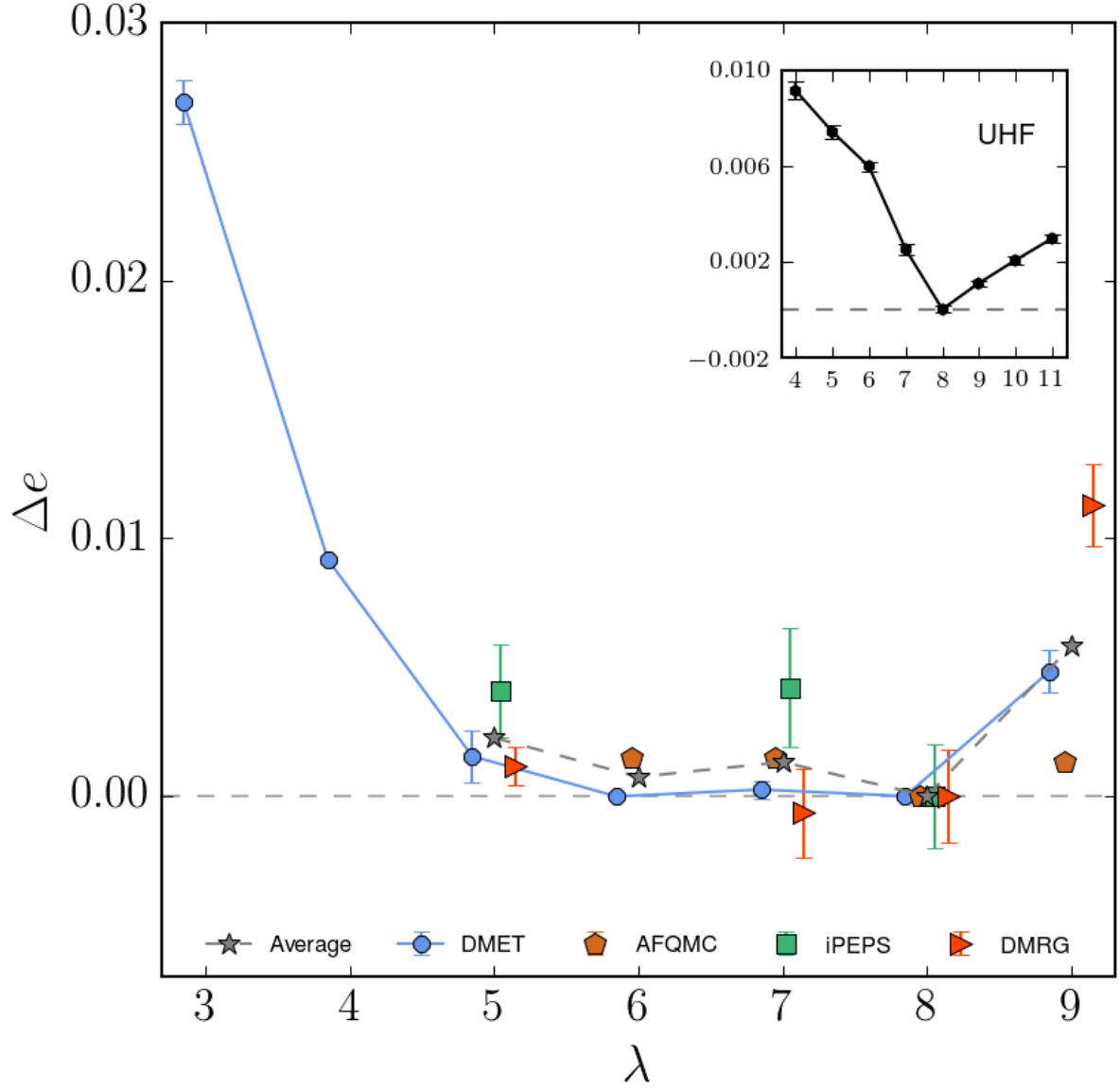


Figure 3: Energies of stripes with different wavelengths relative to that of the wavelength 8 stripe from DMET, AFQMC, iPEPS and DMRG. To aid readability, the data points are shifted horizontally. Inset: Relative energies of stripes with different wavelengths from UHF, with an effective coupling  $U/t = 2.7$ .

$\lambda$  for the multiple methods. Earlier DMRG calculations on the Hubbard model had focused on  $\lambda = 4$  (half-filled stripes) which are seen in HTSC's (13, 14), but we now observe that these are relatively high in energy. A striking feature is that for  $\lambda = 5 - 8$  the energies are nearly degenerate. This is clearly seen in the DMET data where stripes of all wavelengths can be stabilized, as well as the plot of the averaged energy of the methods between  $\lambda = 5 - 8$ . The energy difference between the  $\lambda = 5$  and  $\lambda = 8$  stripe in the different methods is estimated to be between  $0.0005t$  (DMRG)– $0.0041t$  (iPEPS). This suggests that the magnetic domain walls can fluctuate freely, consistent with proposals for fluctuating stripes. In particular, the stripes may be distorted at small cost over long length scales.

Although the different wavelengths are nearly degenerate, there appears to be a slight minimum near wavelength  $\lambda = 8$  (a filled stripe) in all the methods. Very recently, similar filled stripes have been reported as the ground state in part of the frustrated  $t$ - $J$  model phase diagram (44).  $\lambda = 9$  appears significantly higher in energy in both DMET and DMRG. In the DMRG calculations, the  $\lambda = 9$  state was not even metastable as boundary conditions and initial states were varied, so the high-energy state shown was forced with a static potential. The AFQMC results show a much weaker dependence on wavelength for longer wavelengths, for example the  $\lambda = 8$  and  $\lambda = 10$  stripe energies per site appear to be within  $0.0015t$ . However, when a mixture of the  $\lambda = 8$  and  $\lambda = 10$  stripe states is set up on a length 40 cluster that is commensurate with both, the state that survives is the  $\lambda = 8$  stripe, suggesting a preference for this wavelength. The increase in energy at wavelengths  $\lambda > 8$  coincides with unfavourable double occupancy of the stripe. This simple interpretation is supported by a mean-field (unrestricted Hartree-Fock (UHF)) calculation with an effective interaction  $U/t = 2.7$  chosen within the self-consistent AFQMC procedure. The mean-field result shows a clear minimum at a wavelength 8 vertical stripe. (Note that this requires the use of an effective  $U$ ; at the bare  $U = 8$ , mean-field theory would produce a diagonal stripe (45)). The correspondence between the energies and

densities in the effective mean-field and correlated calculations suggests that mean-field theory with a renormalized interaction may be surprisingly good at describing the energetics of stripes. However, mean-field theory appears to somewhat underestimate the degeneracy of the stripes as a function of wavelength, particularly at shorter wavelengths.

The stripe order for the  $\lambda = 8$  stripe from the different methods is depicted in Fig. 4. We show the full period (16) for the spin modulation. The stripe is a bond-centered stripe in the AFQMC, DMRG, and DMET calculations. In the iPEPS calculation, the stripe is nominally site-centered. In all the calculations, the width of the hole domain wall spans several sites, blurring the distinction between bond- and site-centered stripes, and we conclude that the energy difference between the two is very small. There is substantial agreement in the order observed by the different numerical techniques, with only some differences in the modulation of the hole and spin-densities.

Note that for even wavelength stripes, the spin wavelength must be twice that of the charge modulation in order to accommodate the stripe as well as the antiferromagnetic order. At odd wavelengths, site-centered stripes appear in all the calculations, and here charge and spin order can have the same wavelength. (This odd-even alternation does not affect the peaks of the structure factor near  $(\pi, \pi)$ , see SI).

*Pairing order, fluctuations, and superconductivity.* A key question is whether pairing order coexists with stripe order. Previous work on the  $t$ - $J$  model with iPEPS found co-existing  $d$ -wave order for partially filled ( $\lambda < 8$ ) stripes. No  $d$ -wave order is found in the Hubbard  $\lambda = 8$  stripe with any technique. However,  $d$ -wave order can be found at other wavelengths. For example, for  $\lambda = 5$ ,  $\lambda = 7$  stripes, iPEPS produces  $d$ -wave order along the bonds (see Fig. 5) with a maximum  $d$ -wave expectation value of 0.026 and 0.021, respectively. DMRG calculations with pinning pairing fields on the boundary for a  $32 \times 4$  cylinder also find  $d$ -wave order, with an extrapolated maximum  $d$ -wave order of 0.025, consistent with the iPEPS results. In the DMET

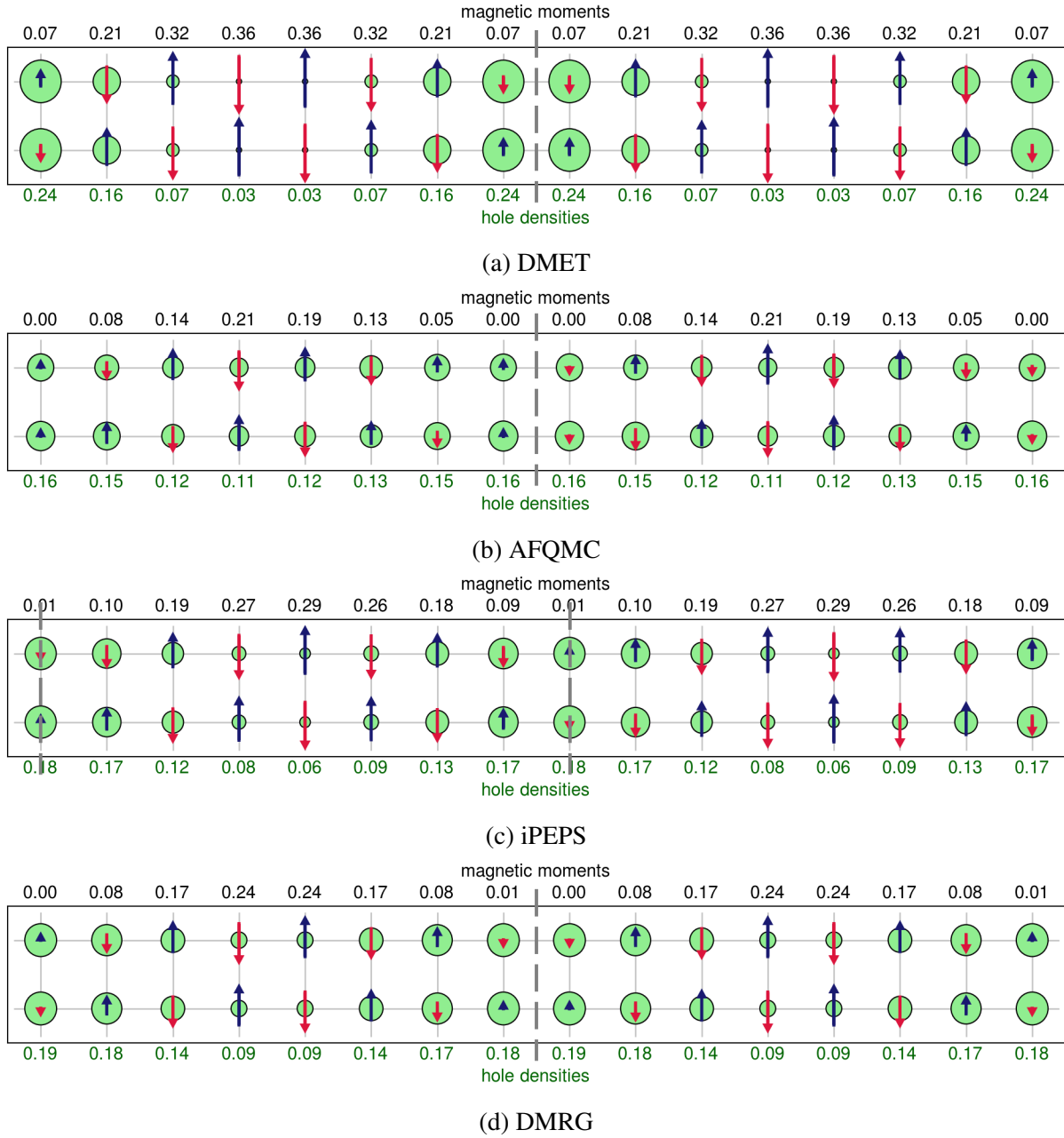
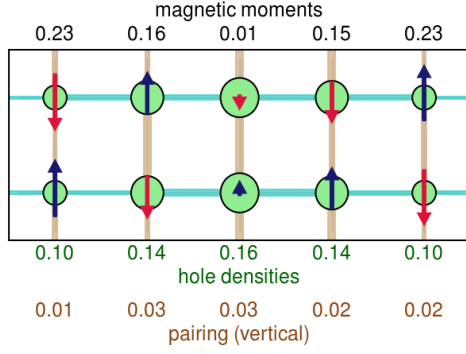
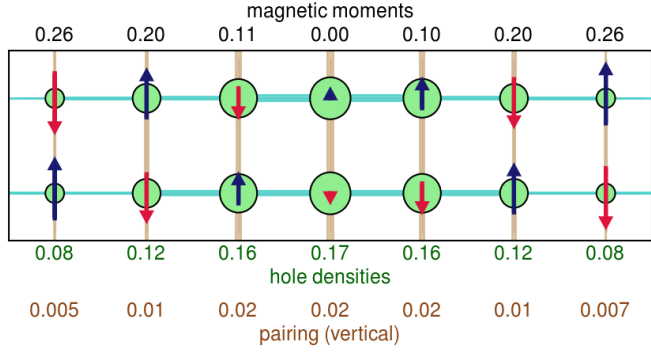


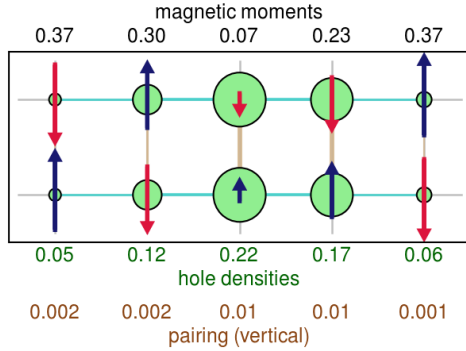
Figure 4: Charge and spin orders in the wavelength 8 stripes from DMET, AFQMC, iPEPS and DMRG. The local magnetic moments and hole densities are shown above and below the order plots, respectively. (Circle radius is proportional to hole density, arrow height is proportional to spin density). The gray dashed lines represent the positions of maximum hole density.



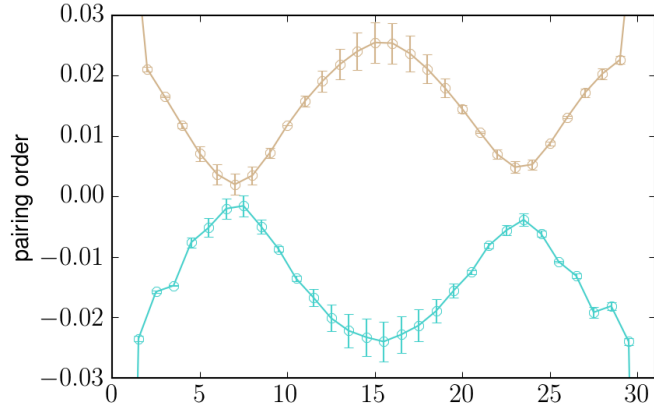
(a) iPEPS  $\lambda = 5$



(b) iPEPS  $\lambda = 7$



(c) DMET metastable  $\lambda = 5$



(d) DMRG pairing order parameters.

Figure 5: Metastable stripe states with  $d$ -wave pairing from iPEPS, DMET, and DMRG. (a)(b) iPEPS stripes with  $\lambda = 5$  and  $\lambda = 7$ . (c) DMET metastable  $\lambda = 5$  stripe with pairing. (Circle radius is proportional to hole density, arrow height is proportional to spin density, bond width is proportional to pairing density). (d) DMRG pairing order parameters on a  $32 \times 4$  cylinder. The positive values are from the vertical bonds and the negative values from the horizontal bonds.



calculations, the lowest energy  $\lambda = 5$  stripe has no  $d$ -wave order, however, at slightly higher energy ( $\sim 0.003t$ ) a  $\lambda = 5$  state similar to the iPEPS stripe can be found with co-existing  $d$ -wave order, but with a substantially smaller maximum order parameter of 0.01. Overall our results support the coexistence of modulated  $d$ -wave order with the striped state, although the strength of pairing is intertwined with the stripe wavelength and filling. The pairing modulation we find (Fig. 5) is in-phase between cells. Other kinds of pairing inhomogeneities, such as pair density waves, have also been discussed in the literature (6).

It has long been argued that fluctuating stripes could promote superconductivity (46–48). Our work provides some support for this picture, as there is a low-energy scale associated with the deformation of stripe wavelength while we also find coupling between the wavelength and the pairing channel. We can imagine fluctuations in wavelength both at low temperatures, as well as in the ground-state. In the latter case, this could lead to a stripe liquid ground-state rather than a stripe crystal. Our calculations are consistent with both possibilities.

*Changing the coupling.* We may also ask whether the  $U/t = 8, 1/8$  doping point is an anomalous point in the Hubbard phase diagram, and, if, for example, moving away from this point would alleviate the unusual stripe compressibility that we see. While it is costly to reproduce the entire set of calculations across the phase diagram, in Fig. 6 we show the energies of various striped states and the uniform state at  $U = 6, 1/8$  doping, computed using AFQMC and DMET. At this coupling, we similarly find that the ground state is a filled striped state with wavelength  $\lambda \approx 8$ . Further, the stripes around wavelength 8 have similar energies, although the stripe order appears slightly less compressible than at  $U = 8$ . The trend is consistent with the state at  $U = 4$  of a more sinusoidal spin-density wave, more delocalized holes, and a more pronounced minimum wavelength (17). Overall, the similarity between  $U = 6$  and  $U = 8$  physics suggests that striped orders with low energy fluctuations of domain walls will remain a robust feature of the physics in the moderate to strongly coupled underdoped region.

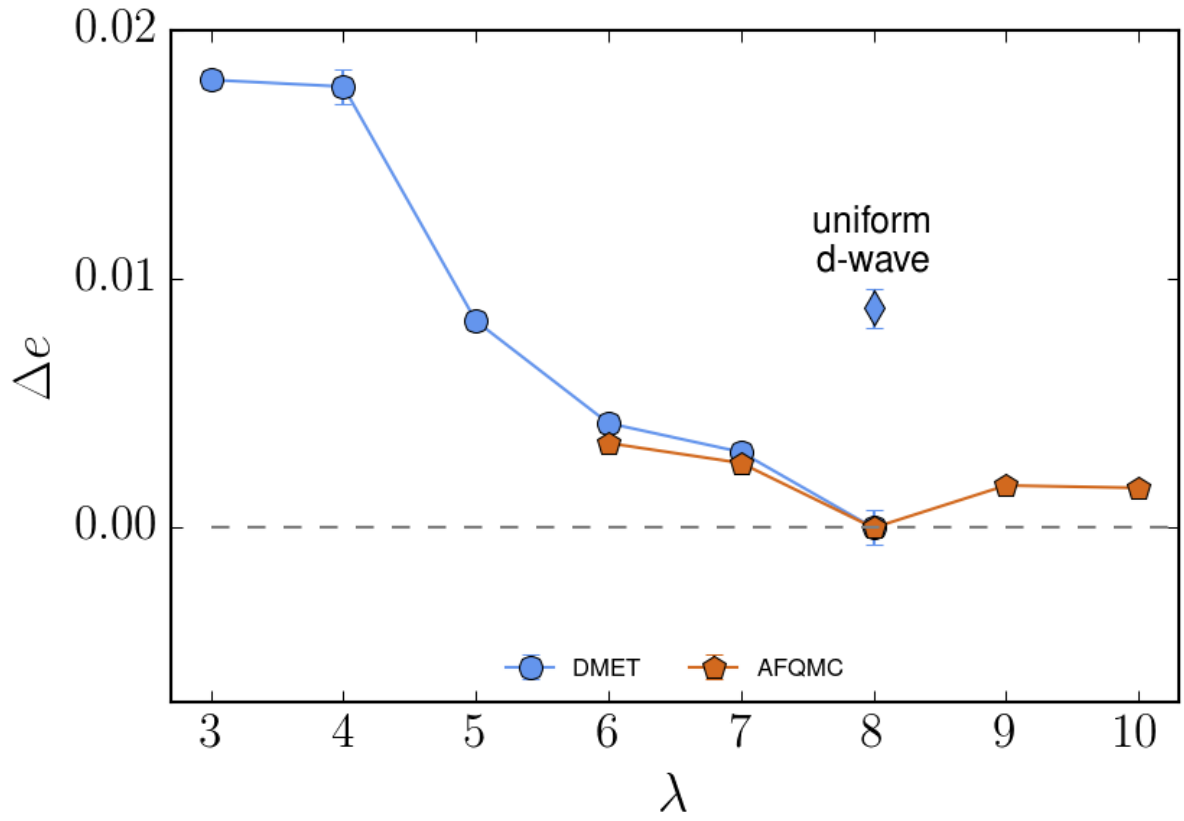


Figure 6: Relative energies of stripe states (vs. wavelength) and uniform d-wave state at  $U/t = 6$  and  $1/8$  doping from DMET and AFQMC.

*Connection to stripe order in HTSC's.* In HTSC's the accepted stripe wavelength at 1/8 doping (e.g. in LaSrCuO) is  $\lambda \approx 4.3$  (close to half-filled) (39). However, we have found the  $\lambda = 4$  stripe is significantly unfavoured in the 2D Hubbard model. This implies that physics beyond the Hubbard model is at play in the charge-ordering of real materials. One possibility is long-range hopping, which has been seen to change the preferred stripe wavelength in the frustrated  $t$ - $J$  model (44). Another possibility is the long-range Coulomb repulsion. Long-range repulsion can play a dual role, in both driving charge inhomogeneity, as well as smoothing it out. In the Hubbard model, where stripes naturally form, the latter property can help drive the ground state towards shorter stripe wavelengths. We have estimated the effect of the long-range interactions on the stripe energetics by computing the Coulomb energy of the charge distributions in Fig. 4. We use a dielectric constant of 15.5 (in the range proposed for the cuprate plane (49)). This gives a contribution favouring the shorter wavelength stripes that is  $\sim O(0.01t)$  per site for the  $\lambda = 4$  versus  $\lambda = 8$  stripe (figure in SI). Although this is only an order of magnitude estimate, it is on the same energy scale as the stripe energetics in Fig. 2, and thus provides a plausible competing mechanism for detailed stripe physics in real materials.

## Conclusions

In summary, in this work we have employed state-of-the-art numerical methods to determine the ground state of the iconic 1/8 doping point of the 2D Hubbard model at moderate to strong coupling. Through careful convergence of all the methods, and exhaustive cross-checks and validations, we are able to eliminate several of the competing orders that have been proposed for the underdoped region in favour of a vertical striped order with wavelength near  $\lambda \approx 8$ . The striped order displays a remarkably low energy scale associated with its wavelength, which implies strong fluctuations either at low temperature or in the ground-state itself. This low energy scale can roughly be described at the mean-field level with a strongly renormalized

$U$ . We find co-existing pairing order with a strength intertwined with the stripe wavelength, indicating a coupling of stripe fluctuations to superconductivity. The stripe degeneracy is robust as the coupling strength is changed.

It has long been a goal of numerical simulations to provide definitive solutions of microscopic models. Our work demonstrates that even in one of the most difficult condensed matter models, such unambiguous simulations are now possible. In so far as the 2D Hubbard model is a realistic model of high-temperature superconductivity, the stripe physics observed here provides a firm basis for understanding the diversity of inhomogeneous orders seen in the materials, as well as a numerical foundation for the theory of fluctuations and its connections to superconductivity. However, our work also enables us to see the limitations of the Hubbard model in understanding real HTSC's. Unlike the stripes at this doping point in real materials, we find filled stripes rather than near half-filled stripes. The physics giving rise to half-filled stripes must therefore arise from terms beyond the Hubbard model, such as long-range Coulomb interactions. These will give contributions larger than the remaining inaccuracies in our simulations. The work we have presented provides an optimistic perspective that achieving a comprehensive numerical characterization of these more detailed models of the HTSC's will also be within reach.

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Supplementary information Sections S1-S9. Detailed description of all methods, data, and analysis. Supplementary Tables S1-S7, Figure S1-S34. References 50-76.



# Supplementary Materials for “Stripe order in the underdoped region of the two-dimensional Hubbard model”

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## 1 S1 Structure of the supplementary information

Section 2 contains notes on the figures and main discussion. Section 3 contains a summary of the best energy data used to compare the relative stripe energetics. Section 4 discusses the estimate of the long-range Coulomb effects. The remaining sections describe in detail the calculations performed using AFQMC, DMRG, hybrid DMRG, DMET, and iPEPS.

## 2 S2 Additional information for figures and main discussion

Fig. 1: The plotted energies (units of  $t$ ) correspond to the following specific calculations.

- AFQMC:  $-0.766 \pm 0.001$  from extrapolation to  $\infty$  (in both length and width directions) clusters with pinning fields.
- DMRG:  $-0.7627 \pm 0.0005$  from extrapolation to  $\infty \times 6$  clusters with pinning fields using the hybrid momentum/real-space representation (h-DMRG).
- DMET:  $-0.77063 \pm 0.00001$  from  $8 \times 2$  clusters with spin-flip boundary conditions.
- iPEPS:  $-0.7673 \pm 0.002$  from  $16 \times 2$  supercells with extrapolation to zero truncation error.

Note that the error bars only reflect errors that can be estimated from the calculations themselves, and not all systematic errors.

Discussion of Fig. 2: The metastable DMET state on the  $\sqrt{5} \times 2$  lattice is slightly higher in energy than the ground-state. It is a “stripe-like” state, but appears to be frustrated at this unit-cell size. It is a little hard to estimate the relative energy of this state and the vertical striped ground state as the tilted impurity cluster energies are systematically shifted with respect to the energies of the non-tilted clusters. We estimate the relative energy of the  $\sqrt{5} \times 2$  state as  $E = E_{\sqrt{5} \times 2} - E_{\sqrt{2} \times 2} + E_{2 \times 2}$ , which includes the difference between the  $2 \times 2$  cluster uniform  $d$ -wave state energy and tilted  $\sqrt{2} \times 2$  cluster uniform  $d$ -wave state. This gives an estimate of  $\sim 0.005t$  above the vertical striped state.

Wavelengths of stripes: A key feature of the stripes that we see is that each stripe acts as an anti-ferromagnetic domain wall. As a well-known consequence, at  $1/8$  doping for half-filled stripes, the wavelength associated with the AF periodicity (8) is twice that of the charge periodicity (4).

As an oversimplified but useful characterization of this periodicity, we describe it by labeling the spin pattern along a fixed row, assuming the stripe is width 1:  $\dots \cdot \uparrow\downarrow\uparrow \cdot \downarrow\uparrow\downarrow \cdot \uparrow\downarrow\uparrow \cdot \dots$ . Here the  $\cdot$ 's indicate the positions of the stripes, and the patterns  $\uparrow \cdot \downarrow$  or  $\downarrow \cdot \uparrow$  signify the domain wall nature of the stripe. Consider a charge wavelength which is an odd integer, e.g. 5:  $\dots \cdot \uparrow\downarrow\uparrow\downarrow \cdot \uparrow\downarrow\uparrow\downarrow \dots$ . We see that the ratio of AF and charge wavelengths is one in this case, not two! This odd-even alternation is potentially confusing, particularly if one has non-integer charge periodicity.

However, experimentally, one looks at structure factors, noting peaks near  $(\pi, \pi)$ . The locations of the peaks nearest  $(\pi, \pi)$  do not show any odd/even alternation. To see this note that the shift of the  $k$ -space origin to  $(\pi, \pi)$ , for one particular row, is equivalent to an alternating sign chain  $-1^x$  in the AF pattern, e.g. for charge wavelength 4,

$$\dots \cdot \uparrow\downarrow\uparrow \cdot \downarrow\uparrow\downarrow \cdot \uparrow\downarrow\uparrow \cdot \dots \rightarrow \dots \cdot \uparrow\uparrow\uparrow \cdot \downarrow\downarrow\downarrow \cdot \uparrow\uparrow\uparrow \cdot \dots$$

and for charge wavelength 5

$$\dots \cdot \uparrow\downarrow\uparrow\downarrow \cdot \uparrow\downarrow\uparrow\downarrow \dots \rightarrow \dots \cdot \uparrow\uparrow\uparrow\uparrow \cdot \downarrow\downarrow\downarrow\downarrow \dots$$

In both the even and odd cases, the distance of peaks from  $(\pi, \pi)$  corresponds to an AF “wavelength” of twice the charge wavelength.

### **3 S3 Summary of stripe energy results**

Table 1: Best estimates of energy (per site) of stripes and competing states for  $U/t = 8$ . AFQMC numbers obtained as described in section 5, DMRG numbers obtained as described in section 6, Hybrid (h-) DMRG numbers obtained as described in section 7, iPEPS numbers obtained as described in section 8, DMET numbers obtained as described in section 9. For the AFQMC calculations (pbc) denotes periodic boundary conditions used on both the short- and long-axes of the cylinder. For the DMRG (real-space) calculations, periodic boundary conditions were used along the short axis, open boundary conditions on the long axis. For the h-DMRG calculations, periodic or anti-periodic boundary conditions were used on the short axis, denoted pbc or apbc. SF denotes that the DMET correlation potential in the spin-channel is flipped, doubling the spin wavelength. (Thus the  $8 \times 2$  (SF) pattern in DMET has a charge wavelength of 8 but a spin wavelength of 16.)

Method	Size	Wavelength	Energy ( $t$ )	Error ( $t$ )
AFQMC	$12 \times 8$ (pbc)	6	-0.7653	0.0002
AFQMC	$14 \times 8$ (pbc)	7	-0.7653	0.0002
AFQMC	$16 \times 8$ (pbc)	8	-0.7668	0.0002
AFQMC	$18 \times 8$ (pbc)	9	-0.7655	0.0002
AFQMC	$20 \times 8$ (pbc)	10	-0.7653	0.0002
AFQMC	$\infty \times 4$	8	-0.7680	0.0001
AFQMC	$\infty \times 6$	8	-0.7653	0.0003
AFQMC	$\infty \times 8$	8	-0.7656	0.0004
DMRG	$\infty \times 4$	8	-0.76598	0.00003
DMRG	$\infty \times 6$	5	-0.7615	0.0004
DMRG	$\infty \times 6$	8	-0.762	0.001
DMRG	$\infty \times 7$	7	-0.762	0.001
DMRG	$\infty \times 6$	9	-0.751	0.0016
h-DMRG	$\infty \times 6$ (pbc)	5	-0.76210	0.00005
h-DMRG	$\infty \times 4$ (apbc)	8	-0.76057	0.00007
h-DMRG	$\infty \times 4$ (pbc)	8	-0.7657	0.0003
h-DMRG	$\infty \times 4$ (av.) <sup>a</sup>	8	-0.7631	0.0003
h-DMRG	$\infty \times 6$ (pbc)	8	-0.7627	0.0005
iPEPS	$5 \times 2$	5	-0.7632	0.0018
iPEPS	$7 \times 2$	7	-0.7631	0.0023
iPEPS	$16 \times 2$	8	-0.7673	0.002
iPEPS	$16 \times 16^b$	diag. $4\sqrt{2}$	-0.7581	0.0014
DMET	$2 \times 2$	$d$ -wave	-0.7580	0.0005
DMET	$3 \times 2$	3	-0.7437	0.0009
DMET	$4 \times 2$ (SF)	4	-0.7614	0.00005
DMET	$5 \times 2$	5	-0.7691	0.001
DMET	$6 \times 2$ (SF)	6	-0.7706	0.00007
DMET	$7 \times 2$	7	-0.7704	0.0003
DMET	$8 \times 2$ (SF)	8	-0.7706	0.00001
DMET	$9 \times 2$	9	-0.7658	0.0008
DMET	$2\sqrt{2} \times \sqrt{2}$	$d$ -wave	-0.7620	0.00001
DMET	$5\sqrt{2} \times \sqrt{2}^c$	frustrated	-0.7689	0.0008

Table 2: Best estimates of energy (per site) of stripes and competing states for  $U/t = 6$ . AFQMC numbers obtained as described in section 5, DMET numbers obtained as described in section 9. Other details as above.

Method	Size	Wavelength	Energy ( $t$ )	Error ( $t$ )
AFQMC	$12 \times 8$ (pbc)	6	-0.8684	0.0001
AFQMC	$14 \times 8$ (pbc)	7	-0.8692	0.0001
AFQMC	$16 \times 8$ (pbc)	8	-0.8718	0.0001
AFQMC	$18 \times 8$ (pbc)	9	-0.8701	0.0001
AFQMC	$20 \times 8$ (pbc)	10	-0.8702	0.0001
DMET	$2 \times 2$	$d$ -wave	-0.8679	0.0007
DMET	$3 \times 2$	3	-0.85867	0.00004
DMET	$4 \times 2$	4	-0.85890	0.00004
DMET	$5 \times 2$	5	-0.86836	0.00001
DMET	$6 \times 2$ (SF)	6	-0.87247	0.00001
DMET	$7 \times 2$	7	-0.87363	0.00002
DMET	$8 \times 2$ (SF)	8	-0.87667	0.0007

## 4 S4 Long-range Coulomb interaction

We estimate the long-range Coulomb interaction in the vertical stripes by computing the electrostatic potential energy from charge patterns obtained from the DMET calculations

$$e_{\text{Coul}} = \frac{1}{N_c} \sum_{i \in \text{imp}, j, i \neq j} (h_i - \bar{h})(h_j - \bar{h}) / 4\pi\epsilon_0 \epsilon r_{ij} \quad (1)$$

where  $N_c$  is the number of impurity sites,  $h_i$  is the hole density on site  $i$ , and  $\bar{h}$  is the average

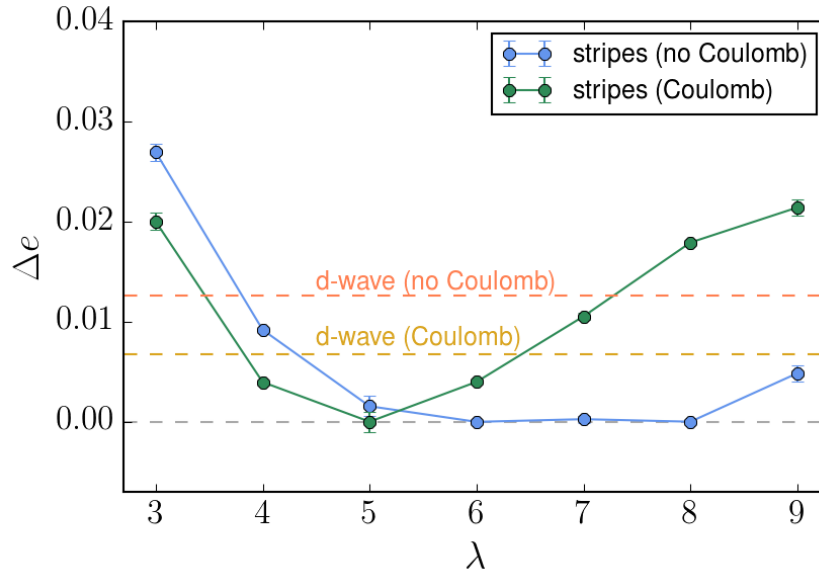


Figure 1: Energy landscape before and after adding the estimated long-range Coulomb interaction for vertical stripes of different wavelength. The charge distributions are from DMET calculations.

hole density ( $1/8$ ). In atomic units, i.e. if we express the energy in Hartrees, and distance in Bohr,  $1/4\pi\epsilon_0 = 1$ . The appropriate dielectric constant to use in a statically screened Coulomb interaction in the  $\text{CuO}_2$  plane has been estimated to lie between about 4 and 27 (49, 50). We use a dielectric constant of  $\epsilon = 15.5$ , and a lattice constant  $a = 3.78\text{\AA} = 7.14$  Bohr corresponding to the lattice constant of  $\text{La}_2\text{CuO}_4$ . We transform the computed Coulomb energy (per site) to units of  $t$ , using  $t \sim 3000K \sim 0.01$  Hartree.

In 2D, the Coulomb summation converges reasonably fast. We choose a cutoff radius as 300 lattice spacings and converge the Coulomb energy to the fourth digit in units of  $t$ . The results for the DMET vertical stripes are shown in Fig. 1. The long-range Coulomb interaction favors shorter wavelength stripes and the homogeneous  $d$ -wave state, shifting the ground state to wavelength 5 and making the uniform  $d$ -wave state also more competitive. Of course the above treatment of the Coulomb term is quite crude, neglects the effect of relaxation in the presence of the Coulomb interaction, and there is significant uncertainty in the dielectric. Nevertheless, the calculation provides an energy scale,  $O(0.01t)$ , over which the long-range Coulomb interaction is important.



## 5 S5 AFQMC calculations

### 5.1 Details of the AFQMC calculations

We studied cylinders of dimension  $l_y \times l_x$  ( $l_x > l_y$ ) with several different boundary conditions. In the first set of calculations, which allow for direct comparison with the finite system DMRG calculations, we used open boundary conditions (OBC) along the  $x$  direction and periodic boundary conditions (PBC) along the  $y$  direction. We also applied pinning fields to pin the underlying spin structures. Several types of pinning fields were used depending on the targeted structure, as shown in Fig. 2. Along each edge, the pinning fields were always anti-ferromagnetic. With FM (AFM) pinning fields, we targeted an odd (even) number of nodes ( $\pi$  phase shifts) in the system ( $l_x$  is always even in our calculations). In some cases, we also applied pinning fields only on one edge to accommodate states with different wavelengths. The strength of the pinning fields is  $|h| = 0.5$  (units of  $t$ ) for all calculations. All these calculations used constrained path AFQMC method with self-consistent optimized trial wavefunctions (51).

In the second set of calculations, we used PBC along both directions, or twist averaged boundary conditions (TABC) along both directions. The twist averaging allows us to reduce the finite size errors in the total energy. These calculations used an unrestricted Hartree-Fock (UHF) trial wavefunction generated by an effective  $U$ . In the following, DMRG results shown for comparison are from section 6. Results are for  $U = 8$  unless otherwise stated.

### 5.2 Wavelength 8 striped ground-state

The spin and hole structure of the  $4 \times 16$ ,  $6 \times 16$ ,  $4 \times 24$ , and  $6 \times 32$  systems are plotted in Figs. 3, 4, 5, and 6 respectively. All the results are obtained with the self-consistent AFQMC method starting from free electron trial wavefunctions.

Exhaustive comparisons were made between AFQMC and DMRG in these systems. The ground state energies for these systems are listed in Table 3. The systematic error compared

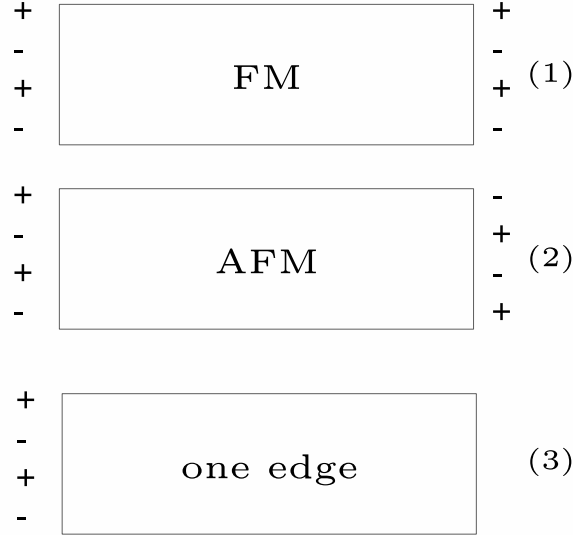


Figure 2: Different types of pinning fields. The relative phase between the pinning fields on the two edges is positive in (1) and negative in (2). We denote (1) and (2) by FM and AFM pinning fields respectively. In some cases, to accommodate states with different wavelengths, we also apply pinning fields on only one edge. We also studied systems with PBC and TABC along both edges, to reduce the finite size effects. Notice that the pinning field along each edge is always anti-ferromagnetic.

with DMRG from the constraint in AFQMC is about  $-0.4\%$ .

For the  $6 \times 16$  system, two different pinning fields, i.e., AFM and FM, were tried. The energy with AFM pinning field (wavelength 8) is lower. For the  $6 \times 32$  system, self-consistent AFQMC finds a ground state structure with wavelength 8 (4 nodes) from a free electron trial wavefunction. We can also construct trial wavefunctions from the density obtained by DMRG. We calculated the energy using the two different trial wavefunctions constructed from the DMRG density for the two states (4 and 6 nodes). The energy comparison of the two stripe states is shown in Table 3. We also did an AFQMC calculation by setting the trial wavefunction as an equal linear combination of the two trial wavefunctions. The state with wavelength 8 survives after convergence. The energy difference between the two states is  $\sim 0.001$  in DMRG and  $\sim 0.003$  in AFQMC. Again the AFQMC energies are slightly lower than the DMRG energies due to the

Table 3: Ground state energies for different systems with pinning fields. DMRG results from section 6.

Size	pinning field	state	DMRG	AFQMC
$4 \times 16$	AFM	2 nodes / wavelength 8	-0.77127(2)	-0.7744(1)
$6 \times 16$ (meta-stable)	FM	3 nodes	-0.7682(3)	-0.7692(1)
$6 \times 16$	AFM	2 nodes / wavelength 8	-0.7691(5)	-0.7725(2)
$4 \times 24$	FM	3 nodes / wavelength 8	-0.76939(3)	-0.7727(2)
$6 \times 32$ (meta-stable)	AFM	6 nodes	-0.7648(3)	-0.7663(1)
$6 \times 32$	AFM	4 nodes / wavelength 8	-0.7658(7)	-0.7691(2)

constrained path approximation. However, the results are consistent (the state with wavelength 8 has lower energy).

After convergence, for all the systems studied, the effective  $U$  in the self-consistent AFQMC calculation is about  $U = 2.7$ .

### 5.3 Comparison of different wavelengths

#### 5.3.1 $4 \times 40$

We studied the  $4 \times 40$  cylinder which accommodates the states with wavelengths of 5 and 8. We used different pinning fields to favor states with different wavelengths.

We applied AFM pinning fields to favor states with an even number of nodes, that is states with wavelengths of 5, 10 or 20. The result from the self-consistent AFQMC with a free trial wavefunction is a state with wavelength 10. If we used a trial wavefunction with wavelength

Table 4: Ground state energies of  $4 \times 40$  system. Pinning fields are applied on only one edge. The energies for the two states with wavelength 8 and 10 are very close, however, when we carry out the AFQMC calculation using the equal linear combination of the two trial wavefunctions as the initial wavefunction, the state with wavelength 8 survives.

pinning field	state	AFQMC
One edge	8 nodes / wavelength 5 (doesn't survive in self-consistent AFQMC)	-0.7657(2)
One edge	5 nodes / wavelength 8	-0.7663(1)
One edge	4 nodes / wavelength 10	-0.7665(3)

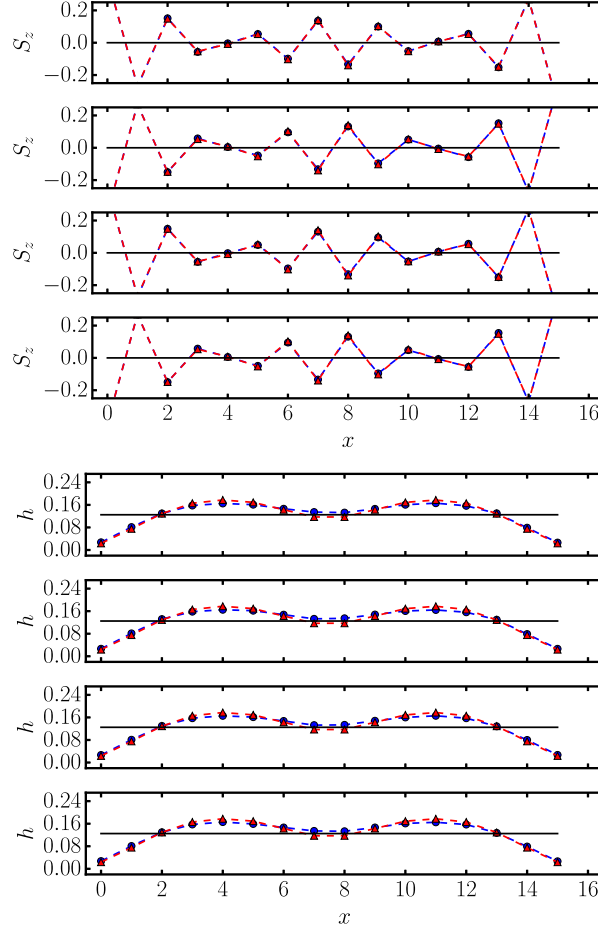


Figure 3: Spin and hole densities along  $l_x$  (with each panel for one value of  $l_y$ ) in  $4 \times 16$  system with AFM pinning fields. Blue circles are for AFQMC and red triangles are for DMRG.

5 (52) to start the self-consistent AFQMC, the final pattern again converged to wavelength 10. This suggests the stripe with wavelength 5 is a higher energy state. The spin and charge patterns are plotted in Fig. 7.

We also tried FM pinning fields with which we obtain the ground state with wavelength 8. The spin and charge pattern are plotted in Fig. 8.

To compare the patterns with wavelength 8 and wavelength 10, we studied the  $4 \times 40$  system with pinning fields on only left edge of the cylinder which accommodates both patterns. We find that the energies for these two trial wavefunctions are very close:  $-0.7665(3)$  for wavelength 10

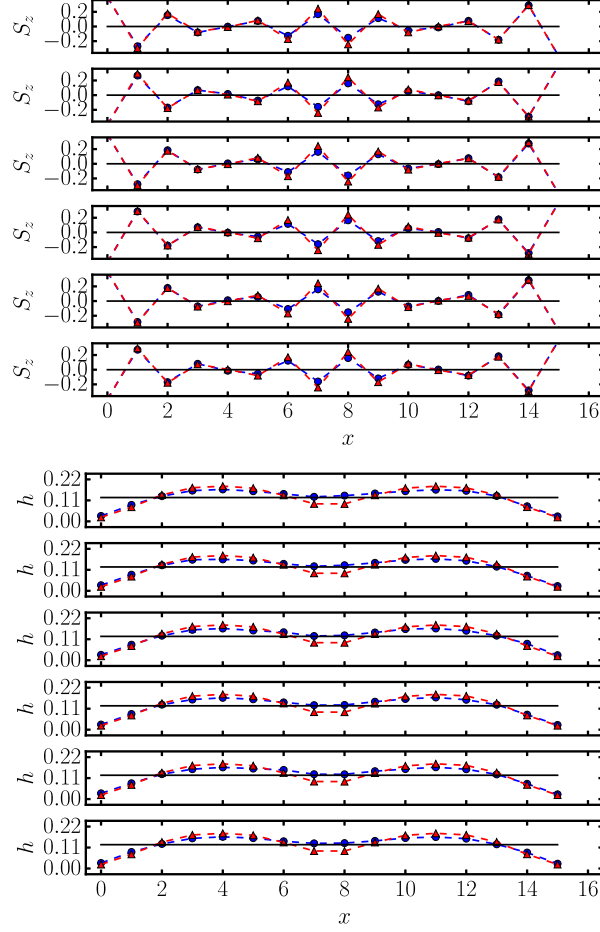


Figure 4:  $6 \times 16$ , with AFM pinning fields. Blue circles are for AFQMC and red triangles are for DMRG.

and  $-0.7663(1)$  for wavelength 8. However, if we use an equal linear combination of the two as the initial wavefunction, the pattern with wavelength 8 survives in the AFQMC calculation. This suggests that the pattern with wavelength 8 is the true ground state. We also calculated the energy of this system using the unstable state with wavelength 5 as the trial wavefunction. The energy is higher:  $-0.7657(2)$ .

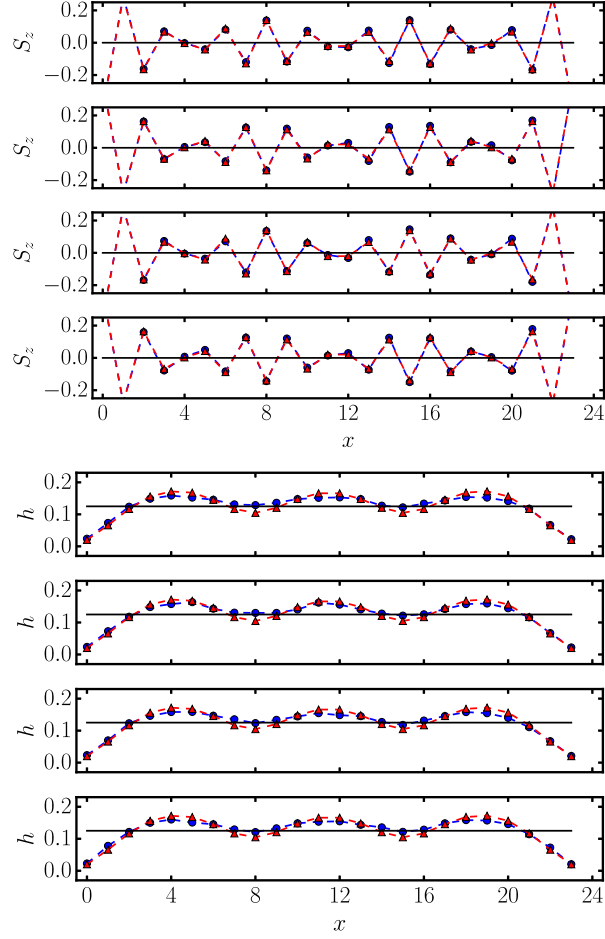


Figure 5:  $4 \times 24$ , with FM pinning fields. Blue circles are for AFQMC and red triangles are for DMRG.

### 5.3.2 $4 \times 48$

We studied the  $4 \times 48$  cylinder which accommodates states with wavelengths of 6 and 8. Unlike the  $4 \times 40$  case, the AFM pinning fields are compatible with both patterns.

From a trial wavefunction with wavelength 8, the self-consistent result is plotted in Fig. 9. The converged state has wavelength of 12 with energy  $-0.7701(1)$ .

The self-consistent result from a free trial wavefunction is plotted in Fig. 10. The converged energy is  $-0.7699(1)$ .

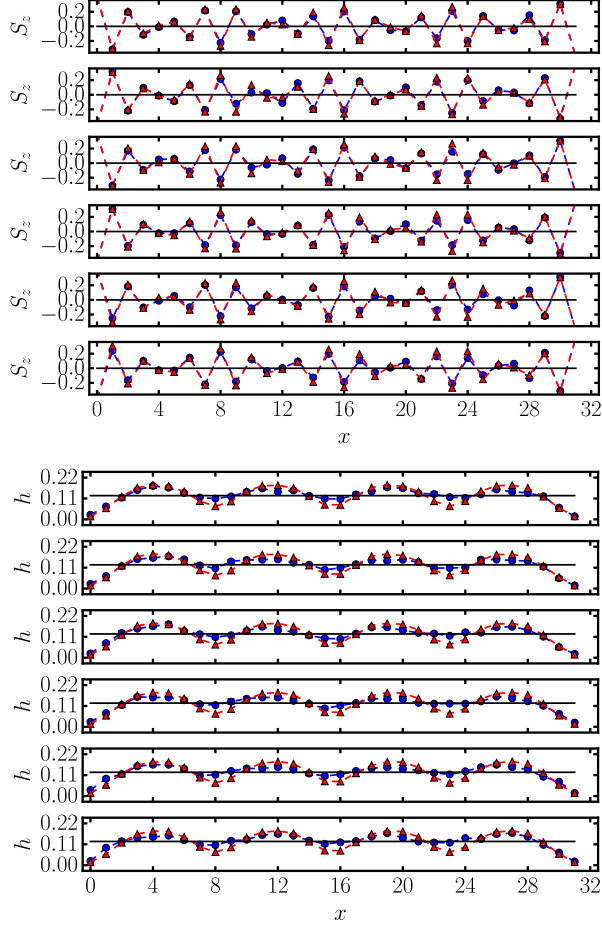


Figure 6:  $6 \times 32$ , with AFM pinning fields. Blue circles are for AFQMC and red triangles are for DMRG.

As in the  $4 \times 40$  case, to compare the two states, we can carry out an AFQMC calculation using an equal linear combination of the two converged trial wavefunctions as a trial wavefunction. After a step of the self-consistent AFQMC calculation, the state with wavelength 8 survives, which indicate, that this state is the true ground state.

We can also construct a trial wavefunction with wavelength 6 (52). With the self-consistent AFQMC calculation this pattern does not survive, but turns into one with wavelength 8 after convergence. For the first few steps when the pattern still has wavelength 6, the energy is  $-0.7693(1)$ , which is higher than the energies of wavelength 8 and 12.

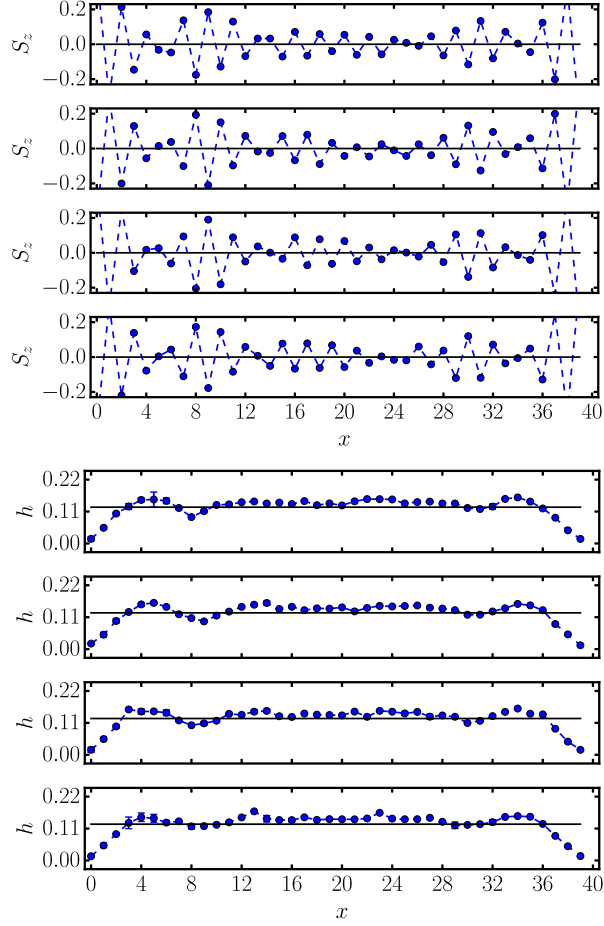


Figure 7:  $4 \times 40$ , with AFM pinning fields. Each panel is for one value of  $l_y$ .

### 5.3.3 $U = 6$ case

We also compared the states with wavelength 7, 9 with 8 using  $4 \times 56$  and  $4 \times 72$  cells for  $U = 6$ . Even though the energies for states with wavelength 7, 9 and 8 are close, the state with wavelength 8 is more robust in the self-consistent AFQMC calculation.

## 5.4 Comparing states using PBC and TABC

From calculations on cylinders in the previous sections, we can estimate an effective renormalized  $U$  for  $U = 8$ ,  $1/8$  doping to be around  $U = 2.7$  (for PBC, we would expect the effective  $U$



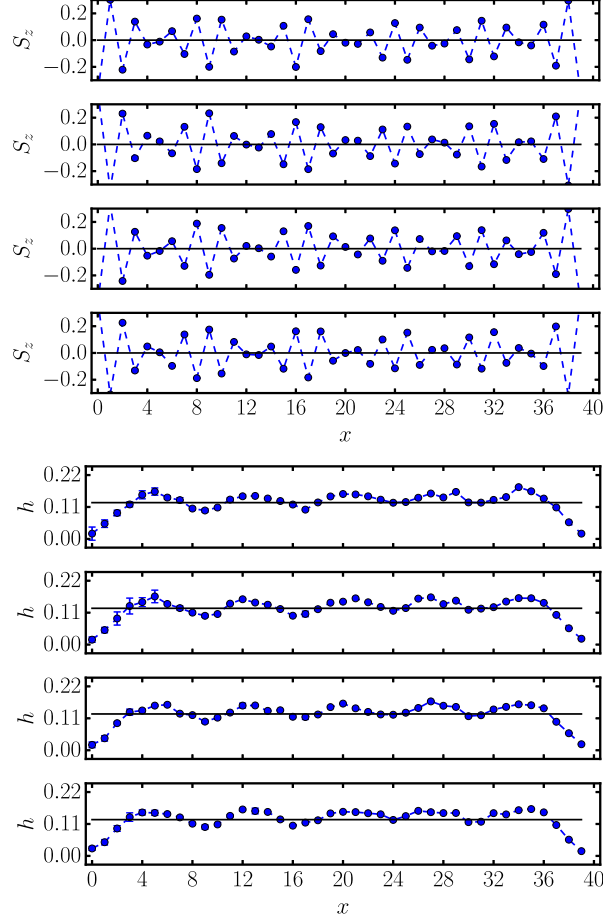


Figure 8:  $4 \times 40$ , with FM pinning fields. Each panel is for one value of  $l_y$ .

to be slightly larger). In this section, we first compare the UHF energies at  $U = 2.7$  for different wavelengths which are shown in the left panel of Fig. 11. Both PBC and TABC are used. With TABC, the finite size effects can be reduced. We use different sizes ( $8 \times 2\lambda$ ) to target states with different wavelengths ( $\lambda$ ). We can find a minimum at wavelength 8 for both PBC and TABC energies.

Next, we use the UHF wavefunctions with  $U = 2.7$  as trial wavefunctions in the AFQMC calculations at  $U = 8$ , using supercells with the same size. The results are plotted in the right panel of Fig. 11. For PBC energies, there is a minimum at wavelength 8. For TABC, the

Table 5: Ground state energies of the  $4 \times 48$  system. AFM pinning fields are applied. The energies for the two stable patterns are very close. However, when we carry out the AFQMC calculation using the equal linear combination of the two trial wavefunctions as the initial wavefunction, the state with wavelength 8 survives.

pinning field	state	AFQMC
AFM	8 nodes / wavelength 6 (doesn't survive in self-consistent AFQMC)	$-0.7693(1)$
AFM	6 nodes / wavelength 8	$-0.7701(1)$
AFM	4 nodes / wavelength 12	$-0.7699(1)$

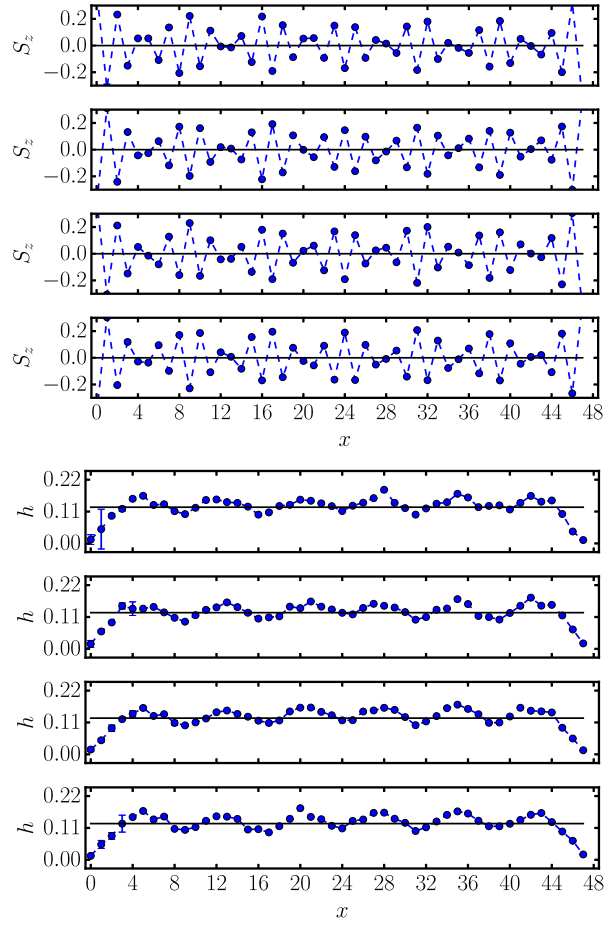


Figure 9: Wavelength = 8 state.  $4 \times 48$ , with AFM pinning fields. A trial wavefunction with wavelength 8 is used in the first step of the self-consistent AFQMC calculation. Each panel is for one value of  $l_y$ .

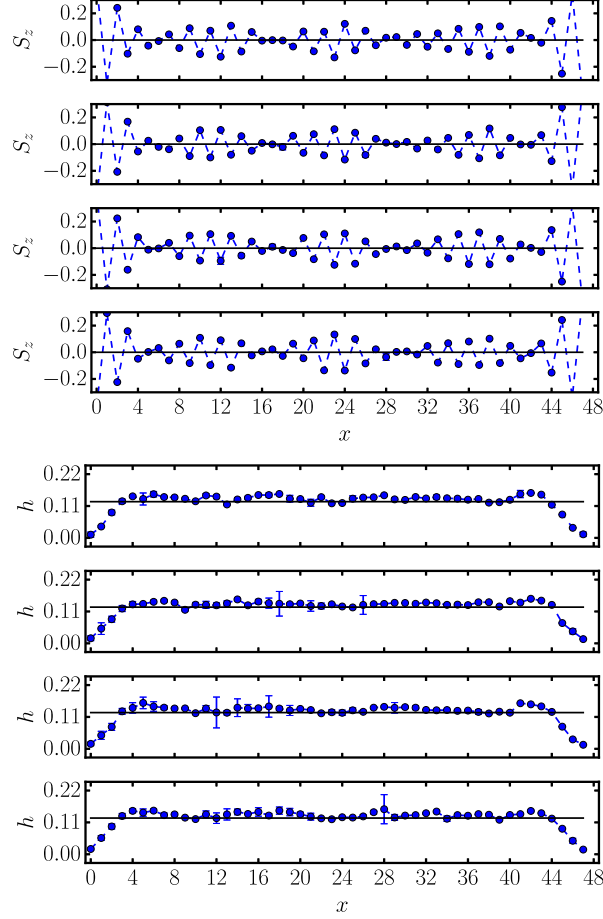


Figure 10: Wavelength = 12 state.  $4 \times 48$ , with AFM pinning fields. Free electron trial wavefunction is used in the first step of the self-consistent AFQMC calculation. Each panel is for one value of  $l_y$ .

energies for wavelength 7, 8, 9 are very close.

## 5.5 Energy of wavelength 8 state at $U = 8$ in the thermodynamic limit

To remove the finite-size effects in the computed ground-state energy for the state with wavelength 8, we extrapolated the energies for systems with length, 16, 32, 48, and 64, and width, 4, 6, and 8. In Fig. 12 it is seen that the energies are indistinguishable for width, 6 and 8 which means the energy is converged to the targeted statistical accuracy with width 6. We also con-

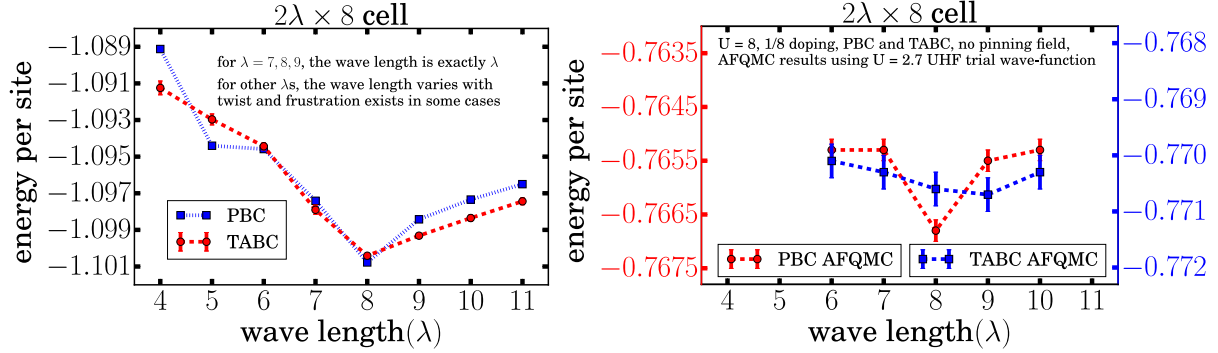


Figure 11: Left: UHF energy with effective  $U = 2.7$ . Right: AFQMC energy of  $U = 8$  using the UHF trial wavefunction in the left panel. The TABC value for wavelength 8, computed here with an UHF trial wavefunction with  $U_{eff} = 2.7$ , is consistent with that from a free-electron trial wavefunction (53). Using a generalized Hartree-Fock (GHF) trial wavefunction gives a slightly improved result of -0.766(1) (54).

firmed the width convergence with length 32 systems. The energies are  $-0.7691(2)$ ,  $-0.7688(2)$ ,  $-0.7691(2)$ , and  $-0.7694(3)$  for width 6, 8, 10, and 12 systems respectively.

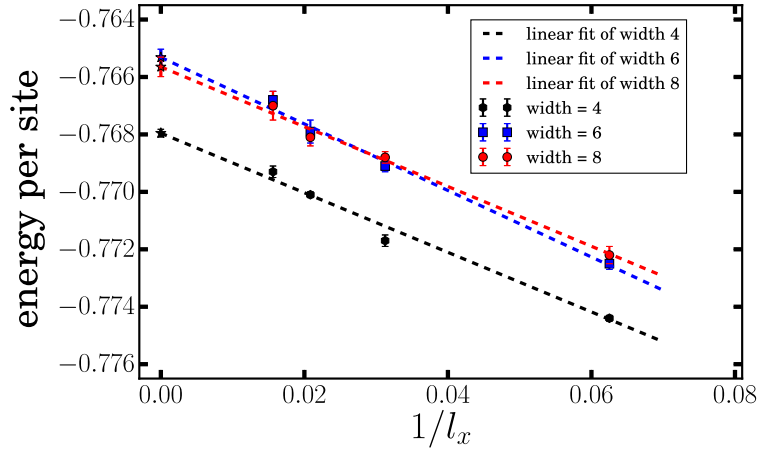


Figure 12: Energies for wavelength 8 state of various lengths and widths for  $U = 8$ . AFM pinning fields are applied. Linear fits of  $1/l_x$  are shown. The infinite length values and error bars from extrapolation are marked as stars in the plot.

size	wavelength	energy
$\infty \times 4$	8	$-0.76598(3)$
$\infty \times 6$	5	$-0.7615(4)$
$\infty \times 6$	8	$-0.762(1)$
$\infty \times 7$	7	$-0.762(1)$
$\infty \times 6$	9	$-0.751(16)$

Table 6: Energies of different stripe states with different wave-lengths on infinite-length cylinders.

## 6 S6 Lattice-basis DMRG

### 6.1 Details of the lattice-basis DMRG calculations

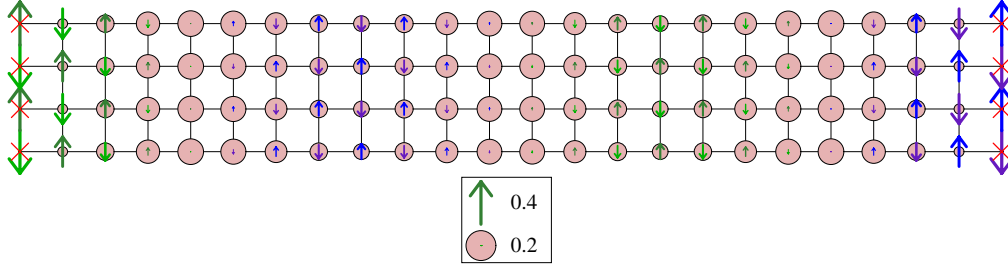
We considered cylinders of size  $L_x \times L_y$  with  $L_x > L_y$ , an open boundary in the  $x$  direction and a periodic boundary in the  $y$  direction. We first considered systems with fixed particle number at  $(1/8)$  doping, and compared the energies of stripe states with different wave-lengths.

We next considered pairing order. To measure the pairing order, we simulated in grand canonical ensemble i.e. without total particle number conservation. The chemical potentials were tuned so that the expectation value of the particle number is close to the desired value ( $7/8$  of the number of sites). We applied pairing fields at the edges, to break total particle number conservation, and observed how the pairing order decays into the bulk.

### 6.2 Fixed particle number

#### 6.2.1 Energy

We summarize the energies of different stripe states on infinite-length cylinders in Table 6. The states of wave-length  $7 \sim 8$  have the lowest energies, and the state of wave-length 5 has a slightly higher energy. The state of wave-length 9 is unstable, with a much higher energy.



24 x 4 system, Vertical PBC's  
 $U/t = 8$ , 12 holes  
 $m = 12000$ , truncated =  $5.67e-06$

Figure 13: Spin (arrow) and hole density (circle) expectation values on a  $24 \times 4$  cylinder. The pinning field is applied to the edge sites (denoted by the crosses).

### 6.2.2 Width-4 cylinders

The cylinder sizes  $8 \times 4$ ,  $16 \times 4$ , and  $24 \times 4$  were considered. The ground state on width-4 cylinders was found to have wave-length 8 (see Fig. 13). To stabilize the state and improve the convergence, we applied magnetic pinning fields on the edges; however the states without pinning fields were first calculated and had the same wave-lengths. The pinning field was chosen to fit the anti-ferromagnetic pattern at the edges, with the strength  $|h| = 0.5$ . Fig.13 shows the spin and hole density expectation values for a  $24 \times 4$  cylinder. The energy extrapolation to infinite length is shown in Fig.14.

### 6.2.3 Width-6 cylinders, wave lengths 5 and 8

Cylinder sizes of  $16 \times 6$  and  $32 \times 6$  were considered. In the width-6 cylinders we found competing states with similar energies for wave-lengths 5 and 8; see Fig.16. The wave-length 8 state has a lower energy. To stabilize the states with particular wavelengths, we used as initial states product states with holes in the desired locations, and applied temporary fields and chemical potentials on the whole system in the first few sweeps. The temporary chemical

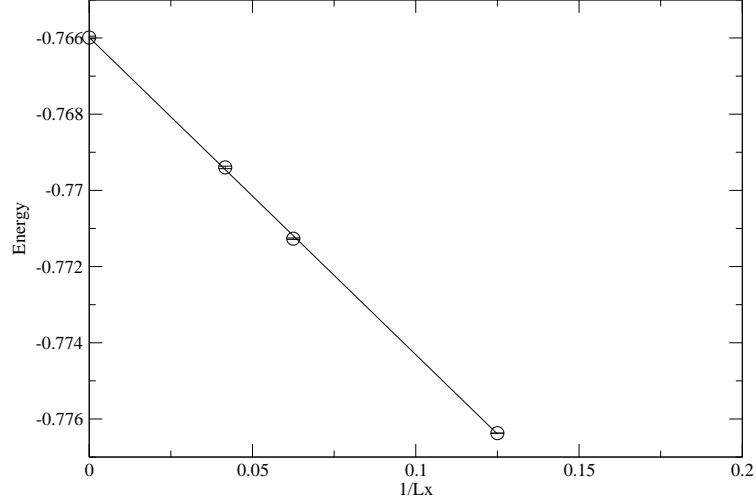


Figure 14: Energy versus  $1/L_x$  for width 4 cylinders.

potential is applied on the sites where the holes are supposed to be in the final striped state, and the temporary field is applied to fit the anti-ferromagnetic domains between holes.

We show the energies versus  $1/L_x$  for the wave-length 5 and wave-length 8 states, both with and without pinning fields, in Fig.15. The spin and hole density expectation values on  $32 \times 6$  cylinders are shown in Fig.16.

#### 6.2.4 Width-7 cylinder, horizontal stripe

To access another possible wave-length, we considered width-7 cylinders, on which horizontal stripe states with wave-length 7 can be stabilized (see Fig.18). We used a product initial state and temporary fields in the first few sweeps, as described in the last section, to stabilize the states. No permanent pinning field was applied. Cylinder sizes of  $16 \times 7$ ,  $32 \times 7$ , and  $48 \times 7$  were considered. The energies for different lengths are shown in Fig.17. The spin and hole density expectation values are shown in Fig.18.

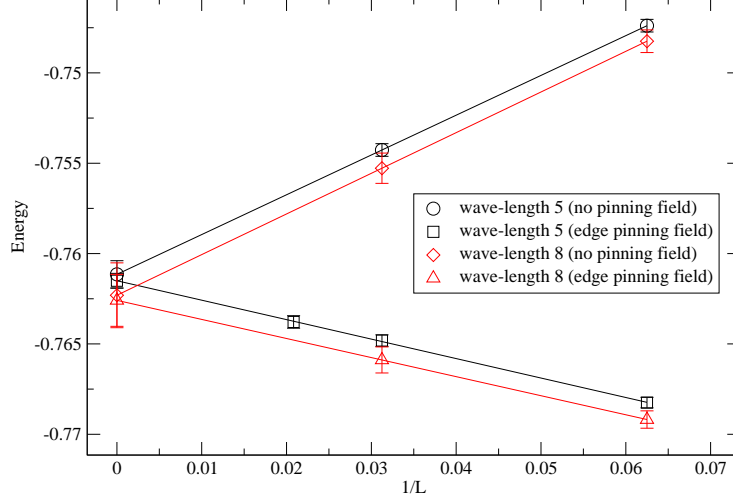
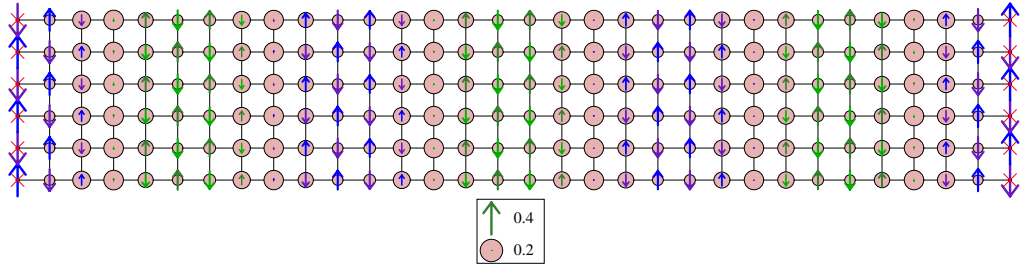


Figure 15: Energy versus  $1/L_x$  for the wave-length 5 and wave-length 8 states on width-6 cylinders. The wave-length 8 state has a slightly lower energy.

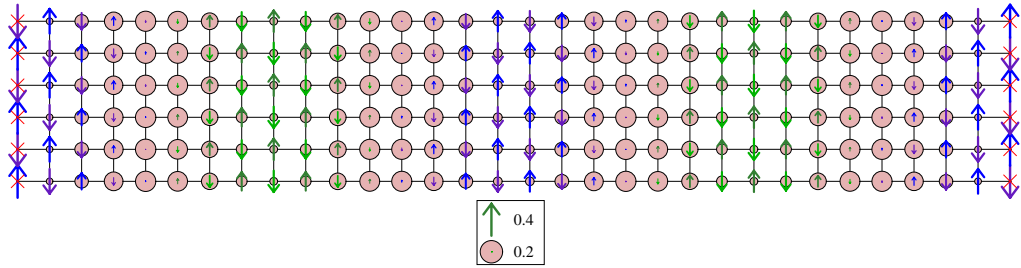
### 6.2.5 Width-6 cylinder, wave length 9

The stripe state with wave-length 9, where each stripe would contain 8 holes, is unstable on a width-6 cylinder (which means that it will split into 4-hole stripes with wave length 5). We therefore provide only a rough estimation of its energy. We forced the holes to be on particular sites by applying strong chemical potentials and magnetic fields throughout the whole system, to form stripes in the first several sweeps up to bond dimension  $m = 4000$ . We then turned off the field except at the edges, and measured the energy in the following few sweeps where the stripes were not yet completely melted. The finite size energy was estimated by the extrapolation of  $m = 7000$  and  $m = 9000$  states, with an error bar defined by the difference between the energy of the  $m = 9000$  state and the extrapolated energy. The energy of the infinite-length cylinder was estimated from the bulk energy by subtracting the energies of  $64 \times 6$  and  $32 \times 6$  cylinders. We show the wave-length-9 stripes with  $m = 5500$  and  $m = 7000$  on a  $32 \times 6$





32 x 6 system, Vertical PBC's  
 $U/t = 8$ , 24 holes  
 $m = 17000$ , truncated =  $2.76e-05$



32 x 6 system, Vertical PBC's  
 $U/t = 8$ , 24 holes  
 $m = 17000$ , truncated =  $6.1e-05$

Figure 16: Spin (arrow) and hole density (circle) expectation values of the wave-length 5 and wave-length 8 states on  $32 \times 4$  cylinders. The pinning field is applied to the edge sites (denoted by the crosses).

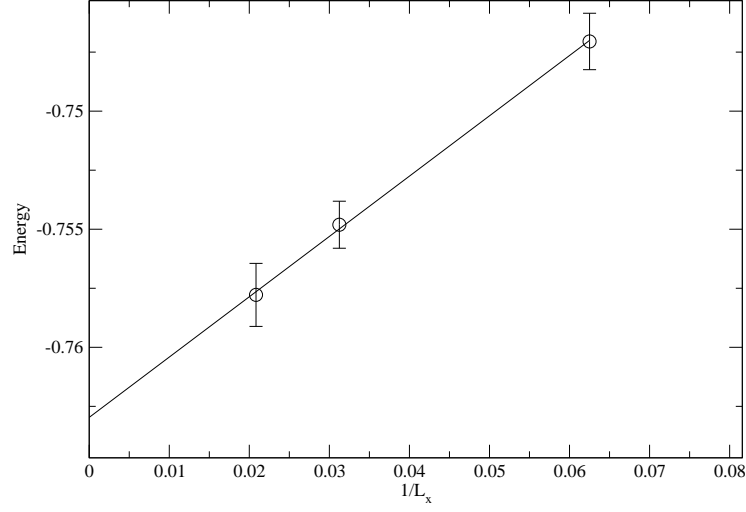
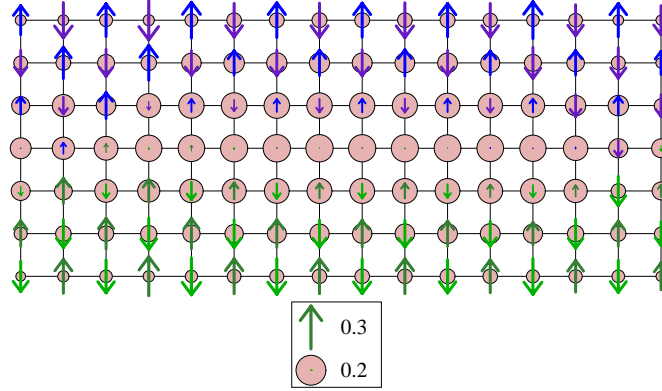


Figure 17: Energy versus  $1/L_x$  for horizontal stripe states of wave-length 7 on width-7 cylinders.



16 x 7 system, Vertical PBC's  
 $U/t = 8$ , 14 holes  
 $m = 17000$ , truncated =  $5.38e-05$

Figure 18: Spin (arrow) and hole density (circle) expectation values for a horizontal stripe state on a  $16 \times 7$  cylinder.

cylinder in Fig.19.

### 6.3 Pairing

Since pairing operators break total particle number conservation, we used grand canonical simulations. An additional global chemical potential term  $-\mu\hat{N}$  was added to the Hamiltonian, where  $\hat{N}$  is the total particle number operator. The chemical potential  $\mu$  is tuned such that  $\langle\hat{N}\rangle$  is close to 7/8 of the number of sites (1/8 doping). Defining the singlet pairing operator  $\hat{\Delta}_{ij}^\dagger \equiv \frac{1}{\sqrt{2}} (\hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow}^\dagger - \hat{c}_{i\downarrow}^\dagger \hat{c}_{j\uparrow}^\dagger)$ , and the averaged pairing operator  $\hat{D}_{ij} \equiv \frac{1}{2} (\hat{\Delta}_{ij}^\dagger + \hat{\Delta}_{ij})$ , we applied d-wave pairing fields  $\mathcal{D}\hat{D}_{ij}$  on the edge bonds, with  $\mathcal{D} = 1.0$  for the horizontal bonds and  $\mathcal{D} = -1.0$  for the vertical bonds, and measured the pairing order  $\Delta_{ij} = \langle\hat{\Delta}_{ij}\rangle$  on each bond for the whole system.

Cylinder sizes of  $16 \times 4$  and  $32 \times 4$  were considered. For both sizes we used a chemical potential of  $\mu = 1.75$ , which gave us charge densities of  $\sim 0.8751$  for the  $16 \times 4$  cylinder and  $\sim 0.8756$  for the  $32 \times 4$  cylinder, for a bond dimension of  $m = 12000$ . The truncation error per site was  $\sim 6 \times 10^{-6}$  for the  $16 \times 4$  cylinder and  $\sim 10^{-5}$  for the  $32 \times 4$  cylinder. The spin, hole densities, and pairing orders are shown in Fig.20.

The pairing orders  $\Delta_{ij}$  on the bonds where  $y = 1$  are shown in Fig.21 (black circles). The positive parts are for the vertical bonds and the negative parts are for the horizontal bonds, showing the *d*-wave symmetry. For the  $16 \times 4$  cylinder, the pairing order strength decays from the edges and has a minimum value  $\sim 0.01$  at the center. For the  $32 \times 4$  cylinder, the pairing order strength decays from the edges, and then grows to a peak at the center. We also show the extrapolated  $\Delta_{ij}$  to zero truncation error in Fig.21 (red diamond). For the  $32 \times 4$  cylinder, when the number of states  $m$  increases, the pairing strength decreases close to the edges ( $x \sim 8$  and 23) and increases in the center, showing the *d*-wave pairing domain. The extrapolations of  $\Delta_{ij}$  for the central bonds ( $i_x = L_x/2, i_y = 1$ ) are shown in Fig.22. Again the positive points are for

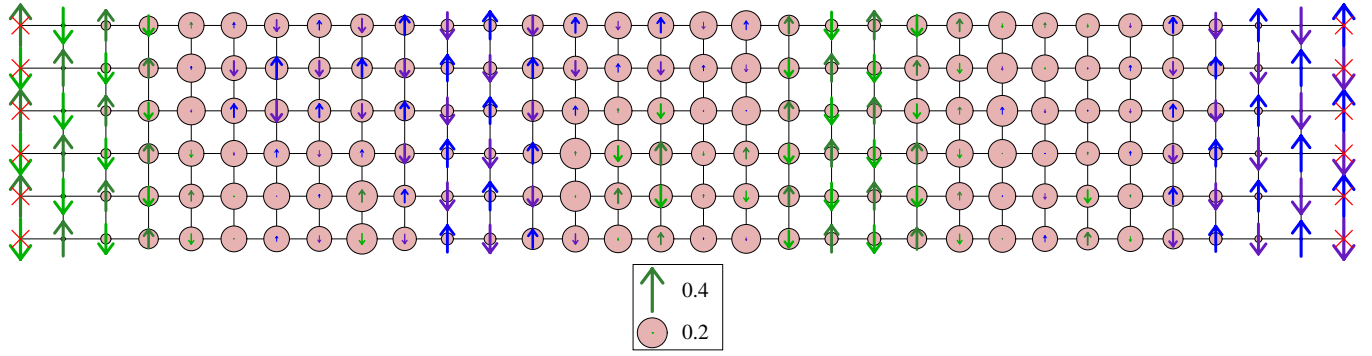
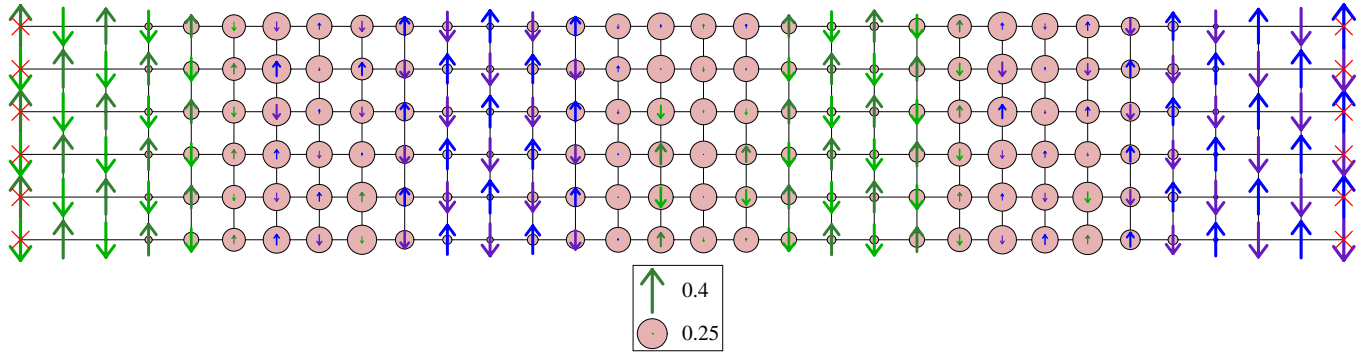
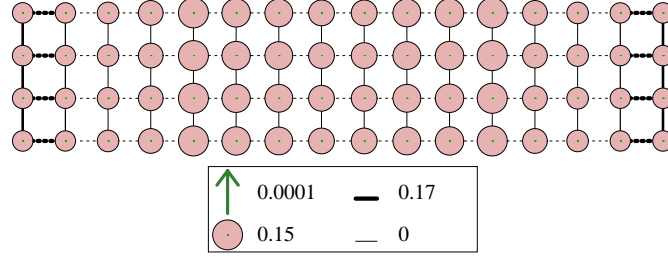


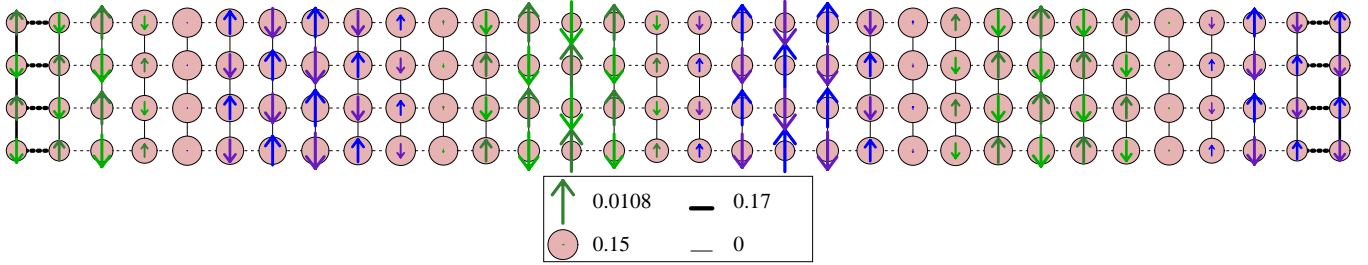
Figure 19: Wave length 9 stripes on a  $32 \times 6$  cylinder for  $m = 5500$  and  $m = 7000$ .

the vertical bonds and the negative points are for the horizontal bonds. We linear extrapolate the last two points, and define the error-bar of extrapolation as  $1/4$  of the difference between the last point and the extrapolated value.

To compare the energy with the results from particle number conserved simulations, we computed the bulk energy  $E_{\text{bulk}} \equiv [E(N_2) - E(N_1)] / (N_2 - N_1)$  for  $N_2 = 32 \times 4$  and  $N_1 = 16 \times 4$ , where  $E(N)$  is the total energy of the system with size  $N = L_x L_y$ . The bulk energy here is  $-0.7639(1)$ . This is a little bit higher than the energy  $-0.76598(3)$  of the infinite cylinder.



16 x 4 system, Vertical PBC's  
 $U/t = 8$ ,  $\mu = 1.75$ , filling = 0.8751  
 $m = 12000$ , truncated = 6.55e-06



32 x 4 system, Vertical PBC's  
 $U/t = 8$ ,  $\mu = 1.75$ , filling = 0.8756  
 $m = 12000$ , truncated = 1e-05

Figure 20: Spin (arrow), hole densities (circles), and pairing order (bonds) in the  $16 \times 4$  and  $32 \times 4$  cylinders. The bond widths are proportional to the strengths of the pairing order  $\Delta_{ij}$ , and the solid lines represent positive signs and dashed lines represent negative signs. The pairing field is applied at the edge bonds, indicated by the thick bonds at the edges.

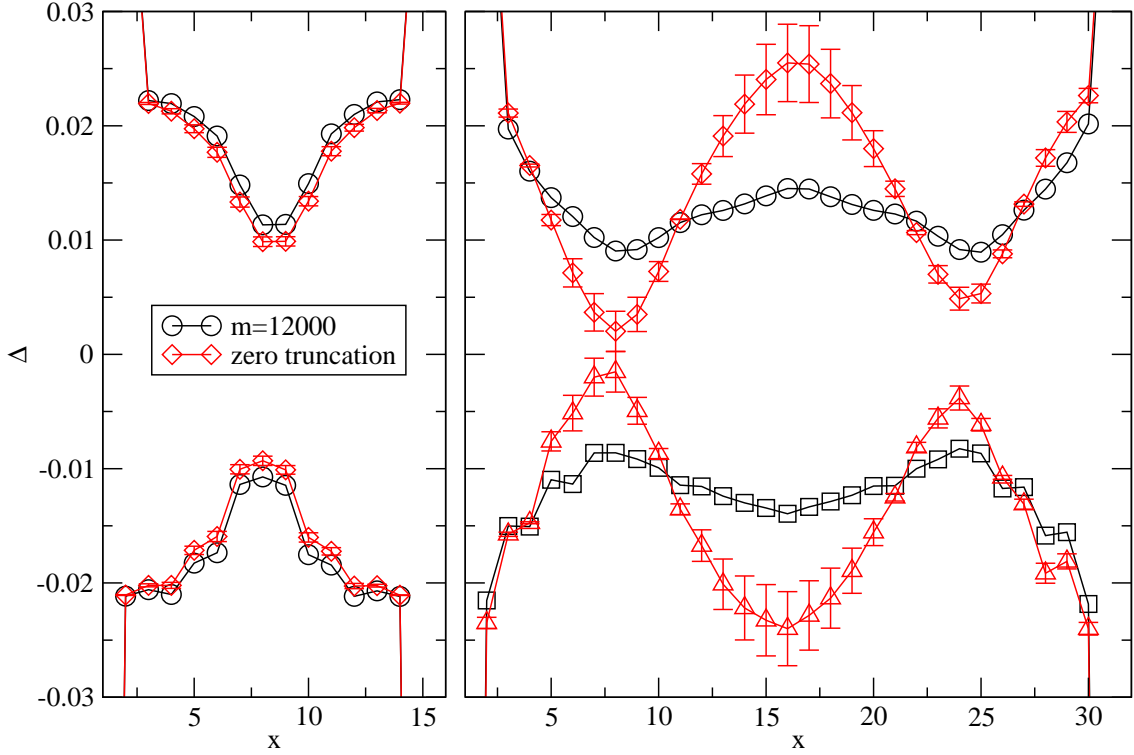


Figure 21:  $\Delta_{ij}$  on bonds of  $y_i = 1$  for the  $16 \times 4$  (left panel) and  $32 \times 4$  (right panel) cylinders. The positive parts are for the vertical bonds and the negative parts are for the horizontal bonds, showing the  $d$ -wave feature. The black circles are measured with bond dimension  $m = 12000$ , and the red diamonds are extrapolated results to zero truncation error. The error-bars are defined as  $1/4$  of the difference between the  $m = 12000$  results and the extrapolated results.

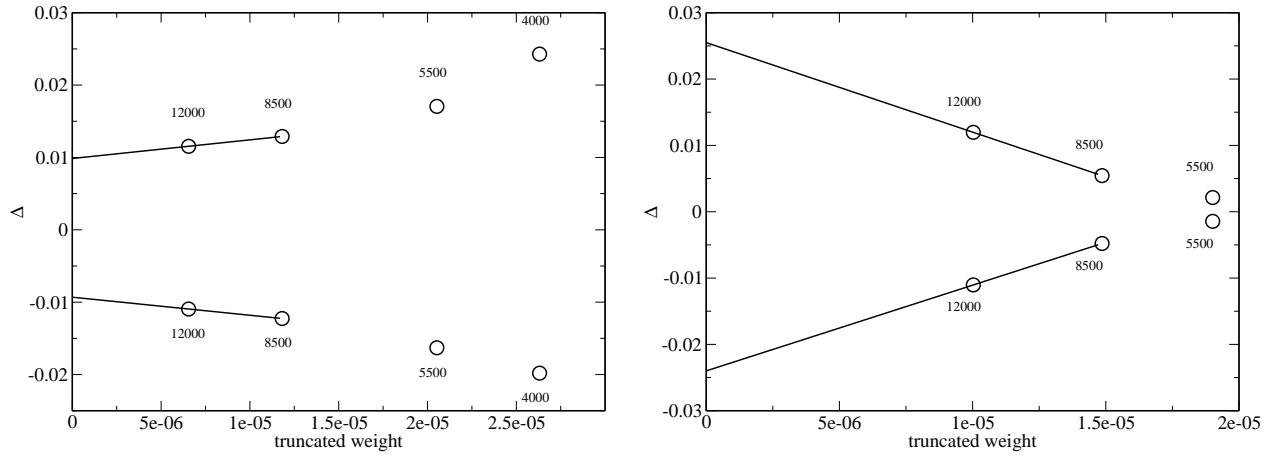


Figure 22: The linear extrapolation of  $\Delta_{ij}$  versus truncation errors for the last two sweeps. Left panel:  $16 \times 6$  cylinder. Right panel:  $32 \times 6$  cylinder.  $i_x = L_x/2$  and  $i_y = 1$ . The positive points are for the vertical bonds ( $j_x = i_x, j_y = i_y + 1$ ) and the negative points are for the horizontal bonds ( $j_x = i_x + 1, j_y = i_y$ ). The numbers show the number of states in each sweep.



## 7 S7 Hybrid-basis DMRG

### 7.1 Details of the hybrid-basis DMRG calculations

We use a cylinder geometry with cylinder length  $L_x$ , width  $L_y$ , with open boundary conditions in the longitudinal (long) axis, and periodic boundary conditions (PBC) or anti-periodic boundary conditions (APBC) in the transverse direction.

We used the density matrix renormalization group (DMRG) algorithm in a mixed–real-momentum-space (hybrid) representation (55). The hybrid-space DMRG algorithm uses a real-space representation in the longitudinal cylinder direction and a momentum-space representation in the transverse direction. The additional transverse-momentum quantum number grants us a speedup over real-space DMRG that grows with the width of the cylinder. For width-6 Hubbard cylinders, the hybrid-space algorithm is approximately 20 times faster than its real-space counterpart.

In order to obtain the ground-state energy for fixed  $L_y$ , we performed consecutive extrapolations first in the DMRG truncation error  $\Delta\xi$  (Fig. 23) and then in the inverse cylinder length  $1/L_x$  (Fig. 24). The ground-state energies for all available combinations of  $L_y$ ,  $L_x$ , boundary conditions, and different stripe patterns (i.e., wavelengths), are given in Table 7.

For width 4, we found stable ground states with 4 holes per stripe for PBC and APBC. For width-6 cylinders with PBC, we found two stable states with 4 and 6 holes per stripe, with the 6-hole stripe pattern being energetically favorable for all cylinder lengths. Thus, for width-4 and width-6 cylinders, we found charge-density stripes with a wavelength of 8 sites for the ground state. For width 6 with APBC, we were not able to effectively stabilize the stripe patterns. For width 8, we did not achieve sufficient convergence in the energy, despite using up to 35 000 states.

In order to directly target and stabilize different stripe configurations on width-6 cylinders

with PBC, we used a sine-shaped pinning field coupled to the local charge density  $n_{xy\sigma}$ ,

$$P = \sum_{xy\sigma} A \cos(k_x x + \phi_0) n_{xy\sigma}, \quad (2)$$

with suitable amplitude  $A$ , wave vector  $k_x$ , and phase  $\phi_0$ . The contribution to the ground-state energy,  $\langle \Psi_0 | P | \Psi_0 \rangle$ , is subtracted after the DMRG calculation. We found a field amplitude of  $A = 0.01$  to be sufficient to stabilize the different stripe patterns and to improve the convergence of the DMRG algorithm.

The stripe patterns in the charge density distribution,

$$\bar{n}_{\text{tot.}}(x) = \sum_{k_y\sigma} \langle \Psi | n_{xk_y\sigma} | \Psi \rangle, \quad (3)$$

can be measured directly and are shown in Figure 25. Depending on the wavelength of the charge density stripes, we also found corresponding peaks in the charge structure factor

$$S_C(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{r}\mathbf{r}'} e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')} \langle n_{\mathbf{r}} n_{\mathbf{r}'} \rangle, \quad (4)$$

with  $n_{\mathbf{r}} = n_{\mathbf{r}\uparrow} + n_{\mathbf{r}\downarrow}$ , shown in Fig. 26 for  $32 \times 4$  and  $32 \times 6$  cylinders; wavelength  $8$  ( $5.\bar{3}$ ) stripes result in peaks at momenta  $k_x = \pm 4/16 \pi$  ( $k_x = \pm 6/16 \pi$ ). Figure 27 shows the corresponding spin-structure factor

$$S_S(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{r}\mathbf{r}'} e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')} \langle m_{\mathbf{r}} m_{\mathbf{r}'} \rangle, \quad (5)$$

with  $m_{\mathbf{r}} = n_{\mathbf{r}\uparrow} - n_{\mathbf{r}\downarrow}$ , which shows peaks at  $k_x = (1 \pm 2/16)\pi$  [ $k_x = (1 \pm 3/16)\pi$ ]. These peaks correspond to the antiferromagnetic order with a modulation / phase-shift of wavelength  $16$  ( $10.\bar{6}$ ). Due to the momentum-space representation in the transverse direction, we could not measure the stripes in the staggered-spin density distribution directly (applying a corresponding field would break the translational invariance).

Finally, we have also measured the decay of the equal-time pair-field correlations

$$D_{y,y}(\mathbf{r}, \mathbf{r}') = \langle \Delta_y^\dagger(\mathbf{r}) \Delta_y(\mathbf{r}') \rangle, \quad (6)$$

with pair-field creation operator  $\Delta_y^\dagger(x, y) = \frac{1}{\sqrt{2}} (c_{x, y+1, \uparrow}^\dagger c_{x, y, \downarrow}^\dagger - c_{x, y+1, \downarrow}^\dagger c_{x, y, \uparrow}^\dagger)$ , as a function of the longitudinal distance for width-4 cylinders (Fig. 28). For small distances  $l_x$ , the correlations decay roughly as  $l_x^{-2}$ , before crossing over to an exponential decay for larger  $l_x$ . The different regimes can be highlighted by choosing a log-log or linear-log scale (Fig. 28 and 29).

Compared to chains or 2-leg ladders the number of states seems insufficient to exactly represent the long-range pair-field correlations for larger correlation lengths. For width 6, the situation becomes even worse, and the exponential decay is dominant at all length scales.

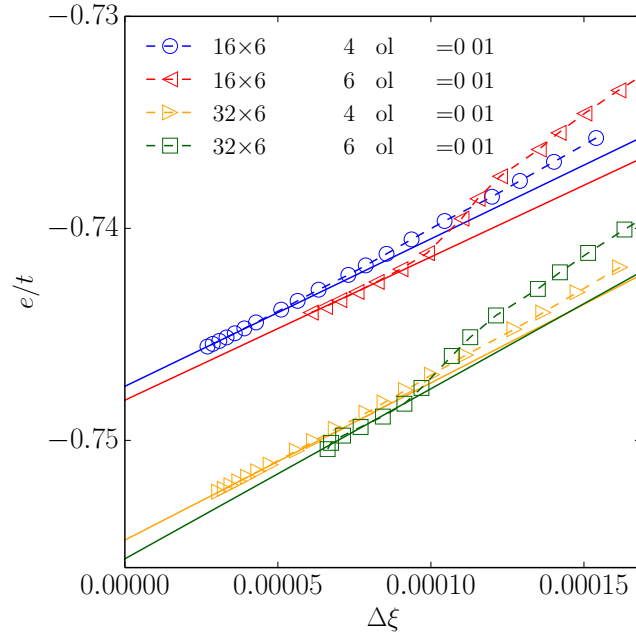


Figure 23: (Color online) Truncation-error extrapolation of the ground-state energy for  $16 \times 6$  and  $32 \times 6$  cylinders, with periodic boundary conditions in transverse direction for 4-hole and 6-hole stripe patterns.

dimensions $L_x \times L_y$	boundary conditions	longitudinal wavelength	holes per stripe	pinning field amplitude	$m_{\max}$	$e/t$
$16 \times 4$	PBC	8.0	4	0	30000	$-0.75114(2)$
$16 \times 4$	APBC	8.0	4	0	30000	$-0.74712(2)$
$32 \times 4$	PBC	8.0	4	0	30000	$-0.75841(2)$
$32 \times 4$	APBC	8.0	4	0	30000	$-0.75382(3)$
$48 \times 4$	PBC	8.0	4	0	27500	$-0.76079(2)$
$48 \times 4$	APBC	8.0	4	0	30000	$-0.75604(4)$
$64 \times 4$	PBC	8.0	4	0	25000	$-0.7621(5)$
$64 \times 4$	APBC	8.0	4	0	27500	$-0.75725(6)$
$\infty \times 4$	PBC	8.0	4	0	-	$-0.7657(3)$
$\infty \times 4$	APBC	8.0	4	0	-	$-0.76057(7)$
$16 \times 6$	PBC	8.0	6	0.01	35000	$-0.7481(2)$
$16 \times 6$	PBC	$5.\bar{3}$	4	0.01	35000	$-0.74745(2)$
$32 \times 6$	PBC	8.0	6	0.01	35000	$-0.7556(7)$
$32 \times 6$	PBC	$5.\bar{3}$	4	0.01	35000	$-0.754702(3)$
$48 \times 6$	PBC	8.0	6	0.01	35000	$-0.7577(3)$
$48 \times 6$	PBC	$5.\bar{3}$	4	0.01	27500	$-0.75727(1)$
$64 \times 6$	PBC	8.0	6	0.01	35000	$-0.7591(2)$
$64 \times 6$	PBC	$5.\bar{3}$	4	0.01	25000	$-0.75842(4)$
$\infty \times 6$	PBC	8.0	6	0.01	-	$-0.7627(5)$
$\infty \times 6$	PBC	$5.\bar{3}$	4	0.01	-	$-0.76210(5)$

Table 7: Zero-truncation-error extrapolated ground-state energies of Hubbard cylinders for  $U/t = 8.0$  at  $n = 0.875$  filling for different stripe patterns, system sizes, and transverse boundary conditions. The given wavelength describes the charge-density waves. For width 6, a pinning field was used to stabilize the different stripe configuration; the energy contribution of the pinning-field was subtracted afterwards.

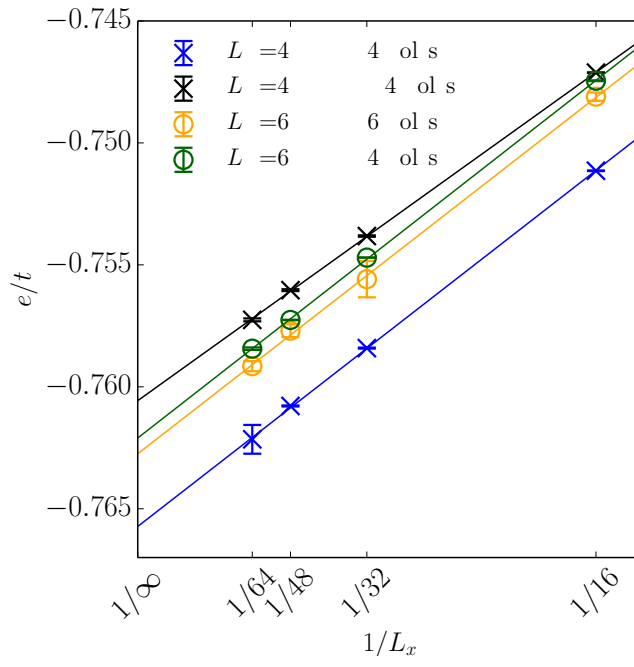


Figure 24: (Color online) Cylinder-length extrapolation of the ground-state energy per cite for cylinders with width 4 and 6.

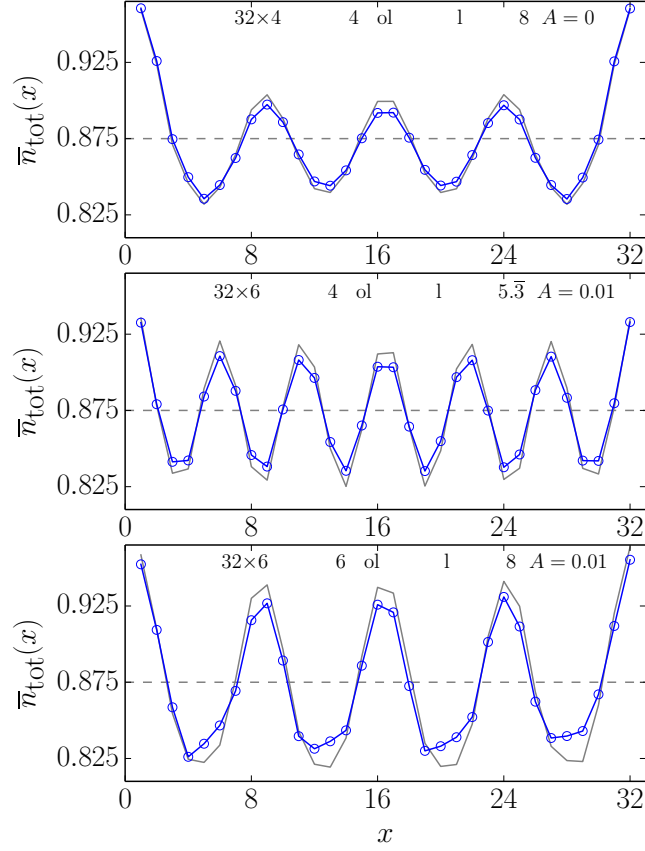


Figure 25: (Color online) Charge density distribution for the 32 $\times$ 4 and 32 $\times$ 6 Hubbard model. The density calculated during the last DMRG sweep is plotted in gray, and the zero truncation error extrapolation is plotted in blue. For width 6 a pinning field with amplitude 0.01 was used to stabilize the stripes.

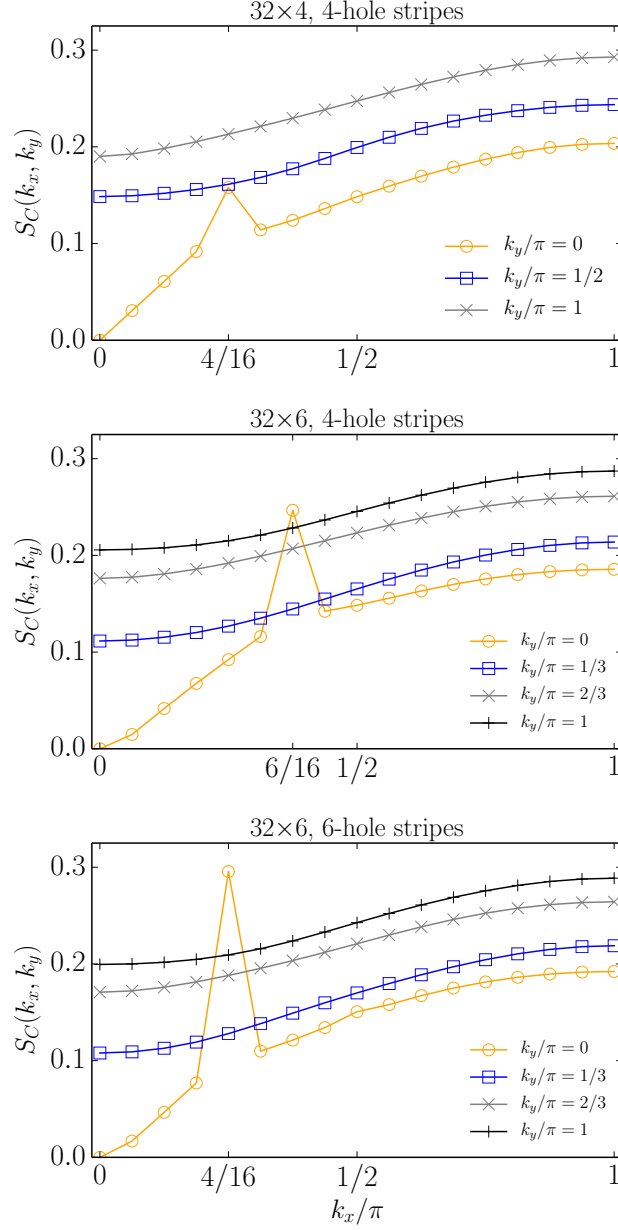


Figure 26: (Color online) Charge structure factor  $S_C(\mathbf{k})$  for width-4 cylinders with 4-hole stripes (top), width-6 cylinders with 4-hole stripes (middle), and width-6 cylinder with 6-hole stripes (bottom). The length of the cylinders in all cases is 32. We show only momenta points  $0 \leq k_{x/y} \leq \pi$ .

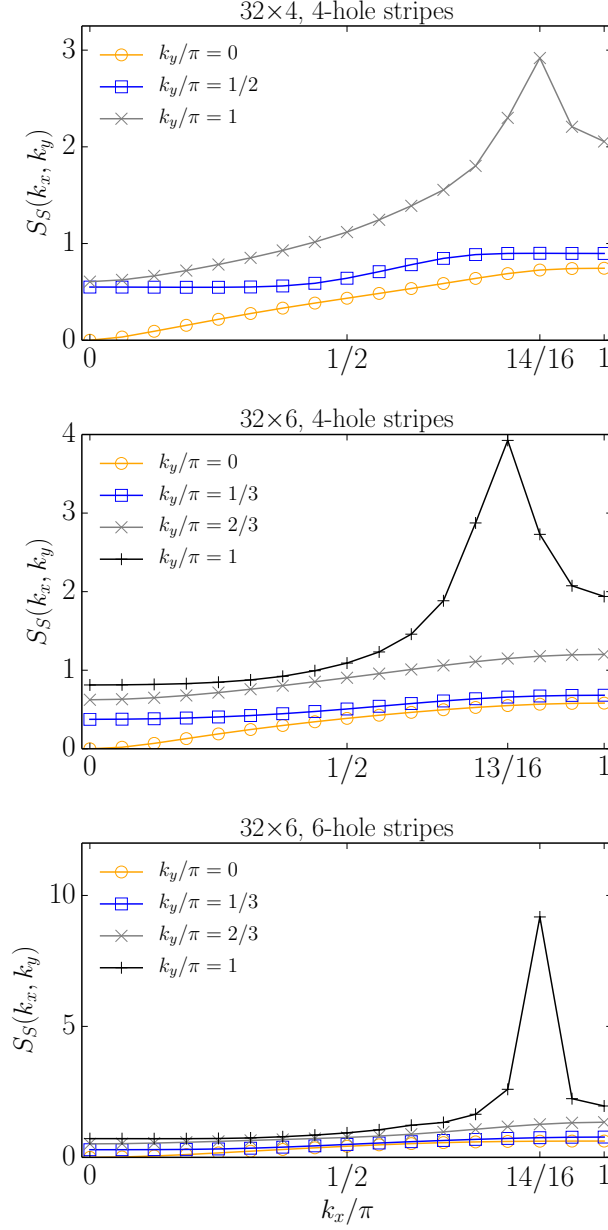


Figure 27: (Color online) Spin structure factor  $S_S(\mathbf{k})$  for width-4 cylinders with 4-hole stripes (top), width-6 cylinders with 4-hole stripes (middle), and width-6 cylinder with 6-hole stripes (bottom). The length of the cylinders in all cases is 32. We show only momenta points  $0 \leq k_{x/y} \leq \pi$ .



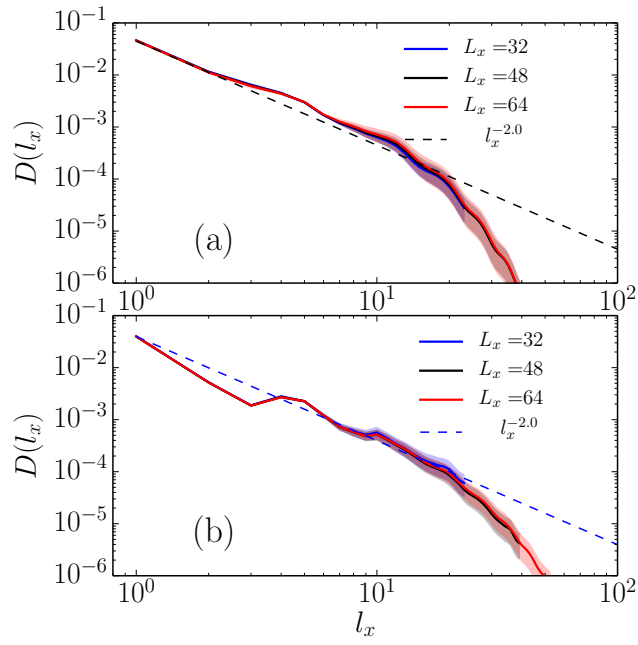


Figure 28: (Color online) Equal time pair-field correlations in longitudinal direction for width-4 cylinders with cylinder length 32 and 48, 4-hole (wavelength-8) stripes, and anti-periodic (top) and periodic (bottom) boundary conditions.

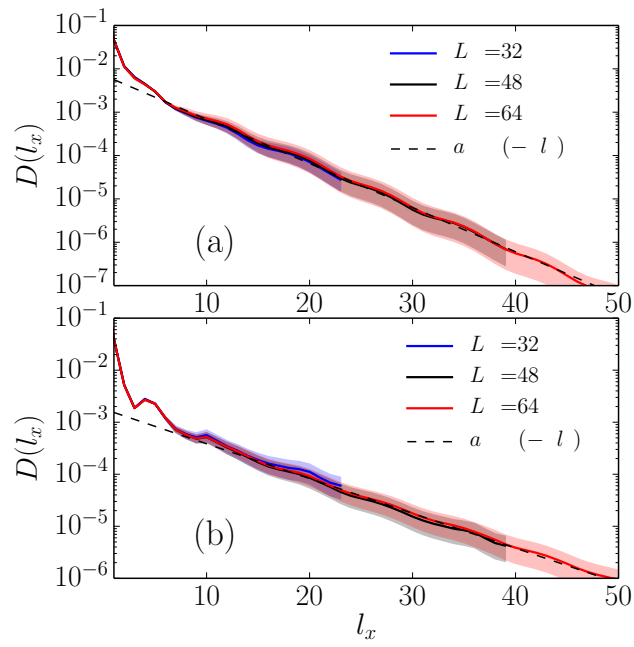


Figure 29: (Color online) Equal time pair-field correlations as in Fig. 28, but on a linear  $x$ -axis.

## 8 S8 iPEPS

### 8.1 Details of the iPEPS calculations

An infinite projected entangled-pair state (iPEPS) (56–58) (also called a tensor product state (59, 60)) is an efficient variational tensor network ansatz for two-dimensional states in the thermodynamic limit which obeys an area law of the entanglement entropy (61). The ansatz consists of a supercell of tensors which is periodically repeated on a lattice, with one tensor per lattice site. Each tensor has a physical index which carries the local Hilbert space of a lattice site and four auxiliary indices which connect to the nearest-neighboring tensors on a square lattice. Each auxiliary index has a certain dimension  $D$ , called the bond dimension, with which the accuracy of the ansatz (the number of variational parameters) can be controlled in a systematic way. An iPEPS with  $D = 1$  corresponds to a product state, and by increasing  $D$  entanglement can be systematically added. In the present work we used bond dimensions up to  $D = 16$  corresponding to highly-entangled states.

For translationally invariant states a supercell with only a single tensor can be used. If the translational symmetry is spontaneously broken, as e.g. in stripe states, a supercell compatible with the symmetry breaking pattern is needed. By running simulations with different supercell sizes we can obtain different competing low-energy states. In order to determine which of these competing low-energy states corresponds to the true ground state a systematic analysis of the energy as a function of  $D$  is required. Here we used the extrapolation technique from Ref. (62) in which the energy is plotted as a function of the so-called truncation error  $w$  in the simulation, and then the extrapolation to the  $w \rightarrow 0$  limit is taken to determine the energy of each of the competing states. While in 2D it is theoretically unknown how the energy depends on  $w$ , several benchmarks (62) have empirically shown that an accurate estimate can be used using a polynomial fit.

In this work the optimization of the tensors has been done using an imaginary time evolution based on the so-called full update (63) (or fast-full update (64)), which is more accurate than the simple update approach (65). Observables are evaluated by contracting the two-dimensional tensor network in a controlled, approximate way, using a variant (66, 67) of the corner-transfer matrix (CTM) method (68, 69). The accuracy of the contraction is controlled by the “boundary” dimension  $\chi$ , which we choose large enough such that the resulting error is small (compared to the effect of the finite  $D$ ). To increase the efficiency we make use of Abelian symmetries (70, 71). Fermionic statistics are taken into account following the formalism explained in Refs (63, 72).

## 8.2 iPEPS results

We have focussed on studying the competition of the stripe states shown in Fig. 30, including vertical width-5 (W5), width-7 (W7), width-8 stripes (W8), and a diagonal stripe state. We find all stripes to be site-centered, not bond-centered. The W5 and W7 stripes exhibit coexisting superconducting order together with CDW and SDW order. The W8 stripe and the diagonal stripe have a period-8 in the CDW order and period-16 in the SDW order. Both states exhibit a filling of exactly one hole per unit length at which superconductivity is vanishing. The typical magnitudes of the local magnetic moments and hole densities of the stripes are given by the black and red numbers in Fig. 30, respectively.

In Fig. 31 we present the results for the energy of these competing states, plotted as a function of the inverse bond dimension and the truncation error  $w$  (62). In order to estimate the energy of each state in the exact limit we extrapolated the data as a function of  $w$  using a third order polynomial. This yields the following estimates for the energies per site, sorted in descending order:  $E_s^{diagonal} = -0.7577$ ,  $E_s^{W7} = -0.7635$ ,  $E_s^{W5} = -0.7637$ , and  $E_s^{W8} = -0.7663$ . By averaging over several fits using different ranges of data points we ob-

tain:  $E_s^{diagonal} = -0.7581 \pm 0.0014$ ,  $-0.7631 \pm 0.0006$ ,  $E_s^{W5} = -0.7632 \pm 0.0018$ , and  $E_s^{W8} = -0.7673 \pm 0.0020$ . We note that the error bar of the  $W7$  stripe is probably underestimated, since inclusion of an additional smaller  $D$  (but less accurate) data point increases the error bar to 0.0023 (but the fit then gets clearly worse in the large  $D$  region). We use this latter value for the error in the main text in order to have a more conservative error bar.

In summary, we find that the width-8 stripe is energetically favored for  $U/t = 8$  and doping  $\delta = 1/8$ .

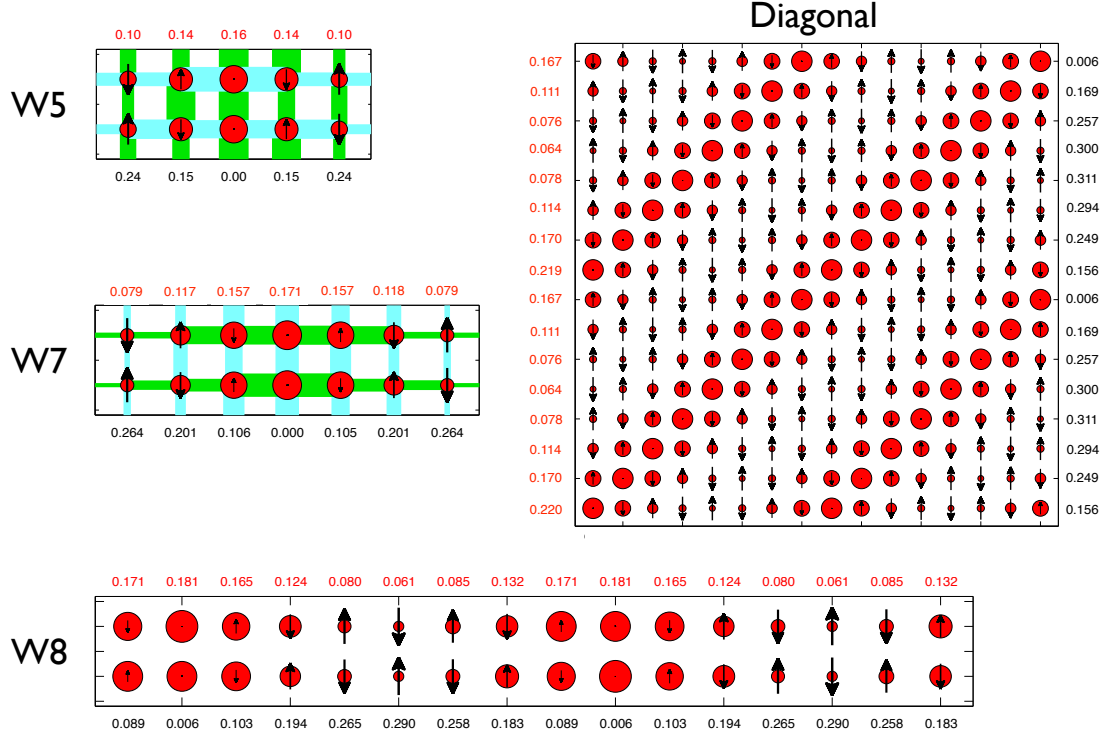


Figure 30: Several competing stripe states obtained with iPEPS for  $U/t = 8$ ,  $n = 1/8$ . The diameter of the red dots (length of the arrows) is proportional to the local hole density (local magnetic moment). The red numbers indicate the hole density, the black numbers the local magnetic moment, averaged over the sites in a column (on a diagonal in case of the diagonal stripe). The width of a bond between two sites scales with the nearest-neighbor singlet pairing amplitude on the corresponding bond with different sign in horizontal and vertical direction illustrated by the two different colors. The width-5 (W5) and width-7 stripes (W7) have coexisting CDW, SDW, and superconducting order. The width-8 stripe has a period-8 in the CDW order and period-16 in the SDW order, and vanishing superconductivity. The diagonal stripe state also has vanishing superconducting order. The pictures have been obtained with bond dimension  $D = 16$ , except for the diagonal stripe state ( $D = 11$ ).

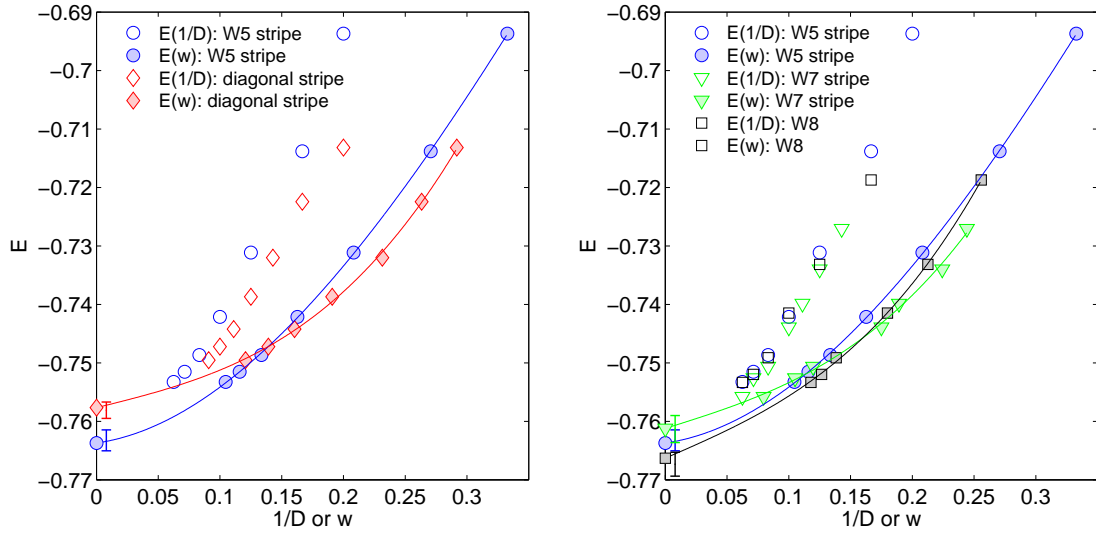


Figure 31: iPEPS results of the energies of the competing stripe states shown in Fig. 30. The data is plotted as a function of  $1/D$  (open symbols) and as a function of the truncation error (filled symbols). The W5-stripe is shown in both panels as a reference. The W8 stripe exhibits the lowest extrapolated energy.

## 9 S9 DMET

### 9.1 Details of the DMET calculations

Density matrix embedding theory (DMET) is a wavefunction-based cluster embedding technique that aims to reproduce the boundary entanglement of an impurity cluster using a set of bath sites. Given an impurity cluster of  $N_c$  sites, DMET maps a large  $L \times L$  lattice to an impurity model through the Schmidt decomposition of an auxiliary lattice wavefunction. The auxiliary lattice wavefunction is usually taken to be of fermionic Gaussian form, i.e. a Slater determinant or BCS state, the ground-state of a quadratic lattice Hamiltonian. The impurity model is then solved with exact or quasi-exact methods such as Lanczos or DMRG to yield an impurity wavefunction. The one-body density matrix of the impurity model and the lattice wavefunction are matched to improve a quadratic correlation potential that is added to the lattice Hamiltonian, which results in a new lattice wavefunction. This process of correlation potential fitting is done self-consistently to optimize the lattice wavefunction and the description of the boundary entanglement. At self-consistency, expectation values both in the cluster and outside can be evaluated using the impurity wavefunction (73, 74).

In this work, we use  $L = 160$  as the linear dimension of the auxiliary lattice, so finite size errors in the auxiliary lattice wavefunction are negligible. We allow the correlation potential, and thus the impurity and auxiliary wavefunctions, to break spin and particle number symmetry. The calculations are similar to those in Ref. (74), but a larger number of impurity cluster sizes, shapes and boundary conditions were explored. Various shapes of impurity clusters are used to accommodate uniform  $d$ -wave order, vertical and diagonal stripes. The shapes of the clusters are summarized in Fig. 32. We do not attempt to do extrapolation of cluster size in this work as in Refs. (74, 75) but compare the energies of different clusters directly. This is making an implicit assumption that the TDL is close to the finite cluster energy, and this lack of TDL extrapolation



is the main systematic error. In our experience, however, it is reasonable to directly compare energies of clusters of the same orientation and family (e.g.  $L \times 2$ ), which is confirmed in this work by comparison with the other techniques.

$\lambda \times 2$  cells [Fig. 32(a)] are used to study vertical stripes with odd wavelengths. As the AF order has a  $\pi$ -phase shift at the domain wall, the AF order is commensurate with the cell size. For even-wavelength stripes, the setup is similar, however, to support a single domain wall, it is necessary for the spin wavelength to be twice that of the charge wavelength. To allow this, rather than using a large cluster of size  $2\lambda \times 2$ , we modify the way the correlation potential is added to the lattice wavefunction, i.e. by swapping the spin channels between neighbouring cells in the longitudinal direction [Fig. 32(c)], so translation by a unit cell gives a time reversal,  $n_{i\uparrow} \rightarrow n_{i\downarrow}$ . Specifically, the local correlation potential in this case is written as

$$u = \sum_{C_1} \sum_{i,j \in C_1} \left( \sum_{\sigma} u_{ij\sigma} a_{i\sigma}^{\dagger} a_{j\sigma} + \Delta_{ij} a_{i\uparrow}^{\dagger} a_{j\downarrow}^{\dagger} + c.c. \right) + \sum_{C_2} \sum_{i,j \in C_2} \left( \sum_{\sigma} u_{ij\bar{\sigma}} a_{i\sigma}^{\dagger} a_{j\sigma} + \Delta'_{ij} a_{i\uparrow}^{\dagger} a_{j\downarrow}^{\dagger} + c.c. \right) \quad (7)$$

where  $C_1$  and  $C_2$  label even and odd cells along the longitudinal  $x$  direction. Both  $\Delta' = \pm\Delta$  possibilities are tested in our calculations, because we cannot determine the phase factor associated with the transformation

$$a_{i\uparrow} \rightarrow a_{i+R,\downarrow}, a_{i\downarrow} \rightarrow \pm a_{i+R,\uparrow}.$$

where the  $R$  denotes translation by a unit cell. As shown in the results, neither parameterization results in finite pairing order in the ground-state of even wavelength stripes.

We also use the tilted clusters in Fig. 32(b) to accommodate diagonal stripes. As the finite-size effects are different in regular and tilted clusters, we use both  $2 \times 2$  and  $2\sqrt{2} \times \sqrt{2}$  clusters to obtain the uniform  $d$ -wave state, to estimate the relative energies of the states on regular and tilted lattices.

In all the calculations reported in this work, the DMRG solution of the impurity problem is

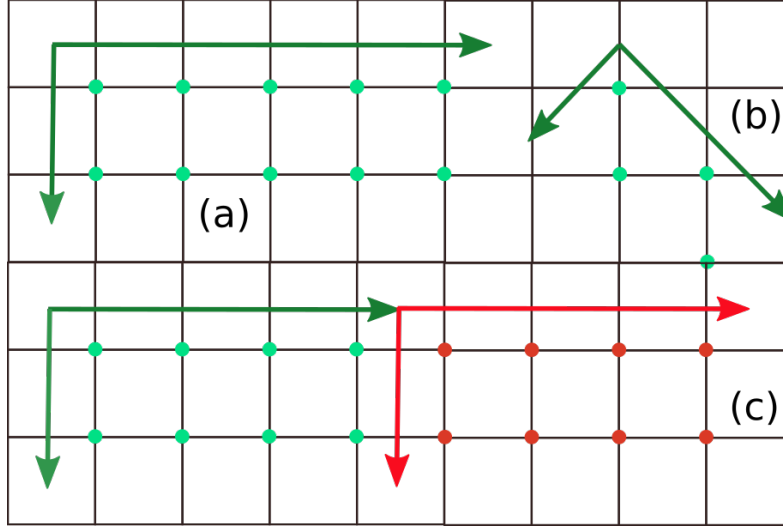


Figure 32: Impurity clusters used in the DMET calculations: (a)  $\lambda \times 2$  clusters. (b)  $\lambda\sqrt{2} \times \sqrt{2}$  clusters. (c)  $\lambda \times 2$  clusters with time inversion on neighboring clusters. Additional data on  $4 \times 4$  clusters is in Ref. (74).

converged in terms of truncation error, and the DMET uncertainty comes from the convergence of the correlation potential. We report the energy and its uncertainty as the average and half of the difference of the last two DMET cycles, respectively.

## 9.2 DMET results

The charge and spin orders of the vertical stripes are plotted in Fig. 33. The corresponding energies are displayed in Table 1. No pairing order is observed at any the wavelengths except for  $\lambda = 9$ . However, for  $\lambda = 9$ , the DMET cycles are significantly harder to converge, indicating frustration in the system. The calculation also results in a much higher energy than the  $\lambda = 8$  calculation.

In addition to the results shown here, we start with random initial guesses for the correlation potential on a  $5 \times 2$  cell, to test the robustness of the solutions. Out of eight different initial guesses, five of them converge to the solution shown in Fig. 33(c); for the other three initial guesses, two of them converge to a stripe with a pair density wave, but with a much higher

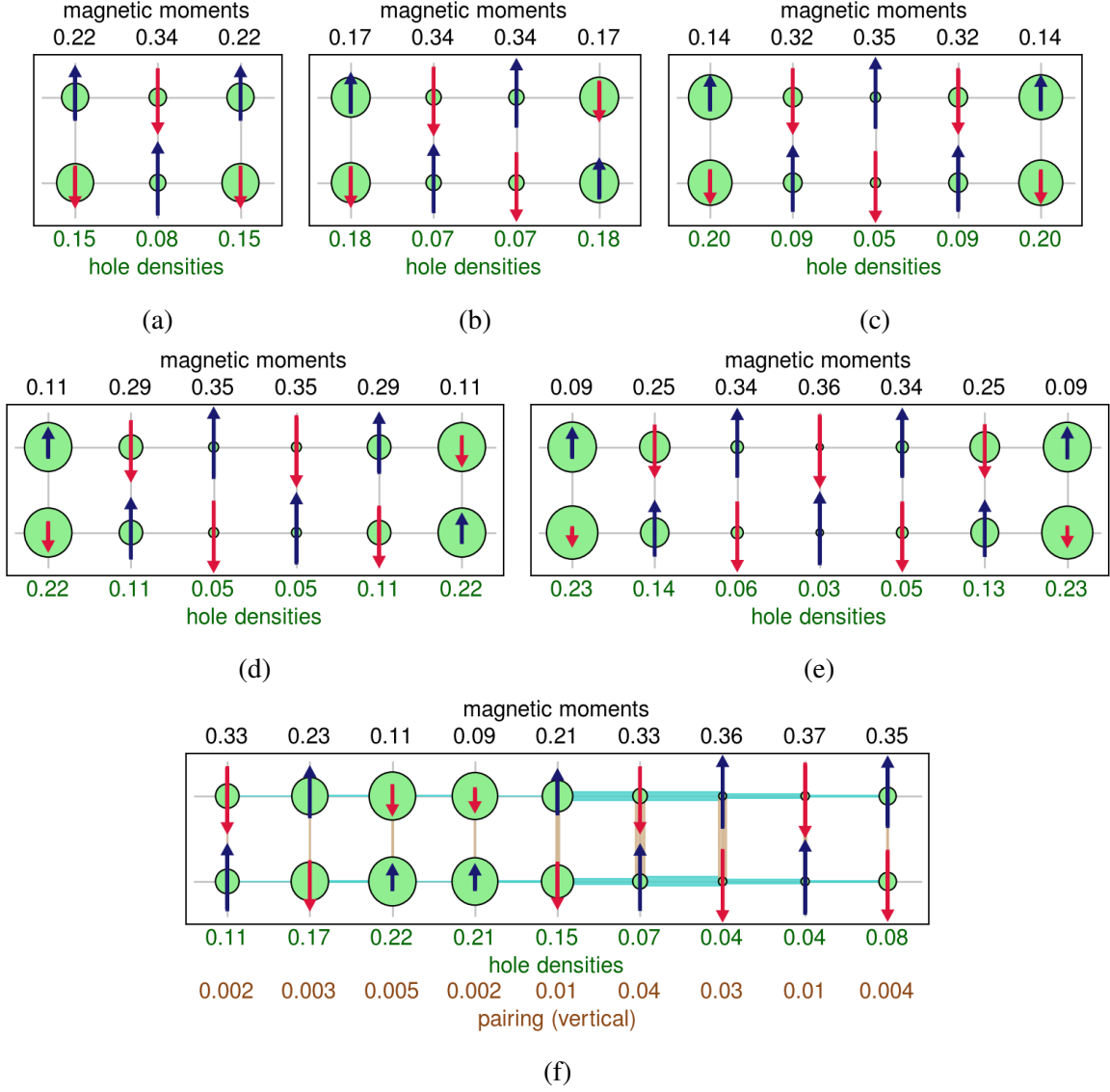


Figure 33: Spin and charge order of vertical stripes or stripe-like states from DMET calculations, for wavelength 3, 4, 5, 6, 7 and 9. The  $\lambda = 8$  state is plotted in Fig. 4(a) in the main text. The spin is flipped between neighboring clusters for the even wavelength stripes.

energy (by  $\sim 0.02t$  per site); one converges to a  $d$ -wave striped state, shown in Fig. 5 of the main text, with only a slightly higher energy ( $\sim 0.003t$  per site).

We use tilted clusters to try to encourage diagonal stripes. Starting from different initial guesses, we obtain two stripe-like states in  $5\sqrt{2} \times \sqrt{2}$  cluster calculations, shown in Fig. 34. To estimate the finite size correction, we use a  $2\sqrt{2} \times \sqrt{2}$  cluster to compute the energy of the uniform  $d$ -wave state, obtaining  $e = -0.76196(1)t$ , compared to  $e = -0.7580(4)t$  in a  $2 \times 2$  regular cluster calculation. Computing a corrected energy of the diagonal striped state to compare to the vertical striped state as  $E = E_{\sqrt{5} \times 2} - E_{\sqrt{2} \times 2} + E_{2 \times 2}$ , we find  $\Delta e \sim 0.005t$  and  $\Delta e \sim 0.036t$  for the two metastable diagonal stripe-like states, relative to the lowest energy vertical striped state.

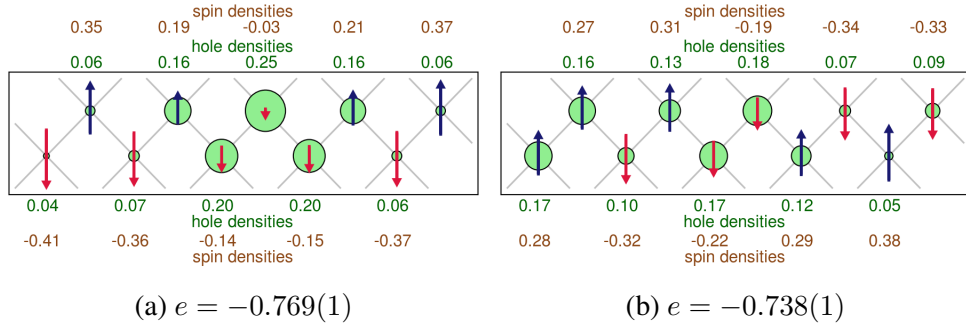


Figure 34: Spin and charge order of stripe-like states with wavevectors along the diagonal direction.

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